Electronic Supplementary Material (ESI) for Dalton Transactions.

Comparing gas separation performance between all known zeolites and their Zeolitic Imidazolate Framework counterparts

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Figure S1. Accessible Surface Area (ASA) plotted against Accessible Volume (AV) for zeolites (red) and their ZIF counterparts (green) in the standard units (for 1.7 Å of probe radius).

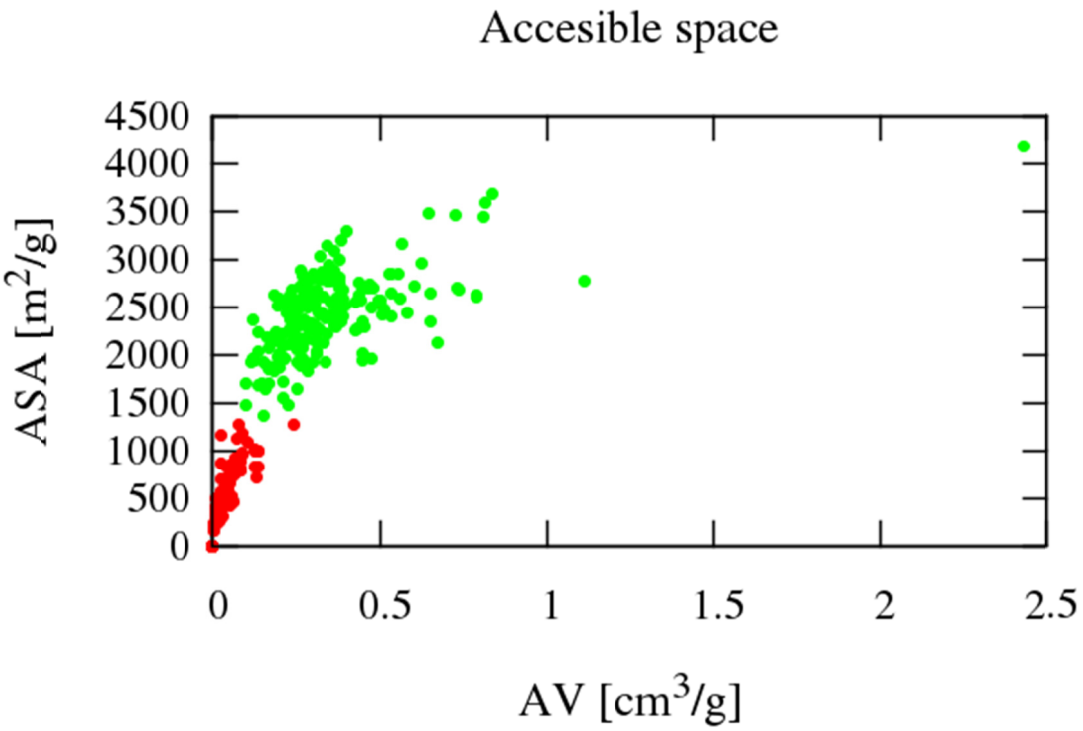
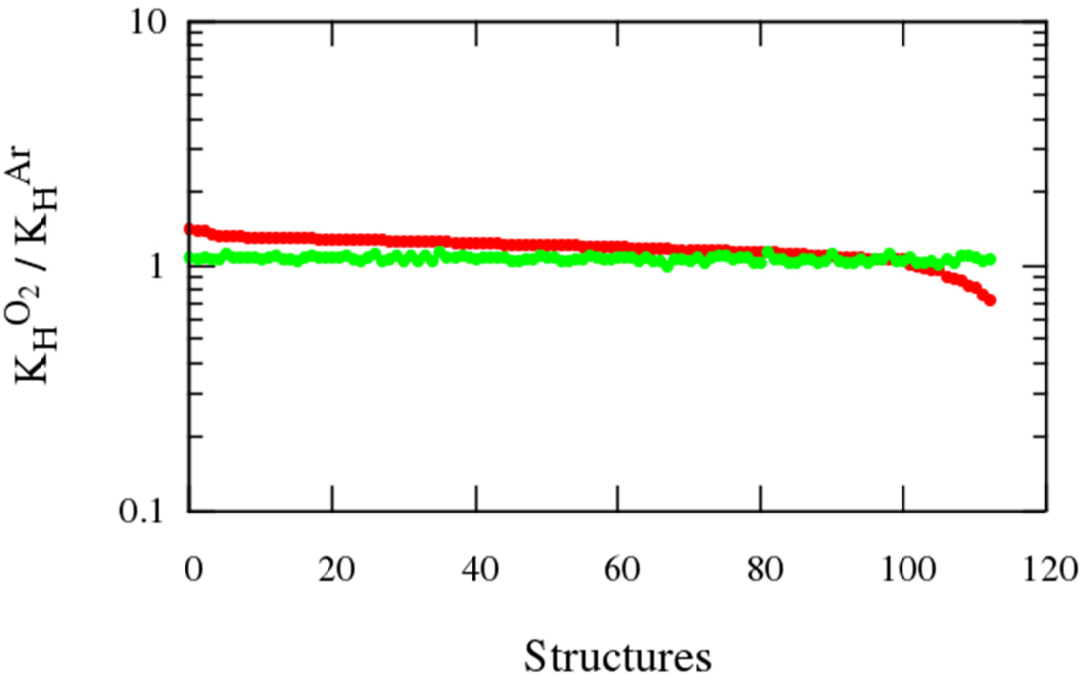


Figure S2. Selectivity of O_2 over Ar at low-coverage regime (ratio of their respective Henry coefficients) for zeolites (red) and their ZIF counterparts (green).



Atomic labels and charges

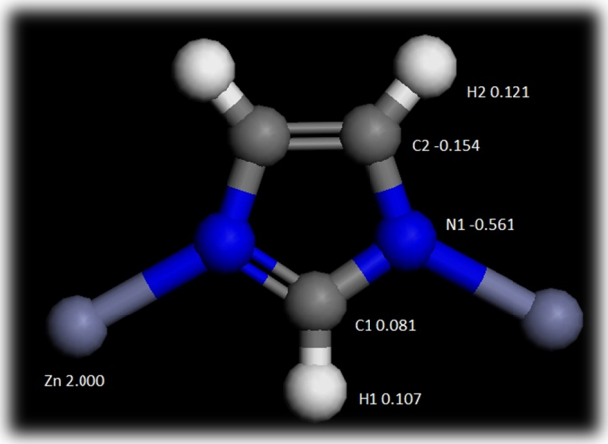


Table S1. Force fields parameters. Imidazole treated as rigid body and positions of the Zn atoms are kept fixed. Atomic labels and charges are displayed in figure above.

Bond stretching (kJ/mol)		
i-j	k_r (kJ/(mol Å^2))	r_0 (Å)
Zn-N	7000	2.02
Bond bending		
i–j–k	k_θ (kJ/mol)	θ_0 (degree)
N-Zn-N	75.00	109.470
Zn-N-C1	127.50	128.362
Zn-N-C2	135.00	125.867

Dihedral			
i–j–k–l	k_Φ (kJ/mol)	Φ_0 (degree)	m
Zn-N-C1-N	5.00	180.00	2
Zn-N-C2-C2	5.00	180.00	2
N-Zn-C1-C2	4.00	180.00	1

Lennard-Jones (Simulations are recommended in several steps to overcome failure caused for too short interatomic distances. Here details for 6 steps, and when i-step fails, insert then two sequentially steps i_a and i_b and back to the planed route)

Common parameters for all steps		
i-j	σ (Å)	ε (kJ/mol)
Zn-Zn	1.9600	0.0523
Zn-N1	2.6050	0.1929
Zn-C1	2.6800	0.1372
Zn-C2	2.6800	0.1372
Zn-H1	2.3050	0.0586
Zn-H2	2.1905	0.0573
N1-N1	3.2500	0.7113
N1-C1	3.3250	0.5059
N1-C2	3.3250	0.5059
N1-H1	2.9500	0.2162
N1-H2	2.8355	0.2113

Lennard-Jones parameters specific for optimization step 1 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	0.1657
	2.6500 a	0.0100 a
	2.6500 b	0.0700 b
H1-H2	2.5355	0.1642
	2.5355 a	0.0100 a
	2.5355 b	0.0700 b
H2-H2	2.4210	0.1628
	2.4210 a	0.0100 a
	2.4210 b	0.0700 b

Lennard-Jones parameters specific for optimization step 2 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	0.3000
	2.6500 a	0.2000 a
	2.6500 b	0.2500 b
H1-H2	2.5355	0.3000
	2.5355 a	0.2000 a
	2.5355 b	0.2500 b
H2-H2	2.4210	0.3000
	2.4210 a	0.2000 a
	2.4210 b	0.2500 b

Lennard-Jones parameters specific for optimization step 3 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	0.5500
	2.6500 a	0.3800 a
	2.6500 b	0.4600 b
H1-H2	2.5355	0.5500
	2.5355 a	0.3800 a
	2.5355 b	0.4600 b
H2-H2	2.4210	0.5500
	2.4210 a	0.3800 a
	2.4210 b	0.4600 b

Lennard-Jones parameters specific for optimization step 4 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	1.0600
	2.6500 a	0.7200 a
	2.6500 b	0.8900 b
H1-H2	2.5355	1.0600
	2.5355 a	0.7200 a
	2.5355 b	0.8900 b
H2-H2	2.4210	1.0600
	2.4210 a	0.7200 a
	2.4210 b	0.8900 b

Lennard-Jones parameters specific for optimization step 5 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	2.0600
	2.6500 a	1.3900 a
	2.6500 b	1.7200 b
H1-H2	2.5355	2.0600
	2.5355 a	1.3900 a
	2.5355 b	1.7200 b
H2-H2	2.4210	2.0600
	2.4210 a	1.3900 a
	2.4210 b	1.7200 b

Lennard-Jones parameters specific for optimization step 6 (a and b denote substeps)

i-j	σ (Å)	ε (kJ/mol)
C1-C1	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-C2	3.4000	0.3598
	3.4000 a	0.0500 a
	3.4000 b	0.1500 b
C1-H1	3.0250	0.1537
	3.0250 a	0.0100 a
	3.0250 b	0.0800 b
C1-H2	2.9105	0.1503
	2.9105 a	0.0100 a
	2.9105 b	0.0800 b
H1-H1	2.6500	0.0600
	2.6500 a	1.3800 a
	2.6500 b	0.7200 b
H1-H2	2.5355	0.0600
	2.5355 a	1.3800 a
	2.5355 b	0.7200 b
H2-H2	2.4210	0.0600
	2.4210 a	1.3800 a
	2.4210 b	0.7200 b

Table S2. Structural information of optimized zeolites.

Zeolite	Lattice constants						Density
	a [Å]	b [Å]	c [Å]	α	β	γ	[kg·m^{-3}]
ABW	9.06	8.53	5.18	90.0	89.3	90.0	1997.5
ACO	9.80	9.80	9.80	90.0	90.0	90.0	1695.2
AEI	13.53	12.48	18.25	90.0	90.0	90.0	1553.8
AEL	8.29	18.26	13.45	90.0	90.0	90.0	1960.5
AEN	17.99	13.62	9.61	90.0	90.0	90.0	2033.6
AET	32.87	14.58	8.39	90.0	90.0	90.0	1785.8
AFG	12.39	12.39	20.67	90.0	90.0	120.0	1743.0
AFI	13.68	13.68	8.46	90.0	90.0	120.0	1744.9
AFN	13.90	13.26	10.16	90.0	107.9	90.0	1792.5
AFO	9.60	25.44	8.27	90.0	90.0	88.7	1975.2
AFR	21.95	13.57	6.94	90.0	90.0	90.0	1544.4
AFS	12.95	12.95	25.96	90.0	90.0	120.0	1481.5
AFT	13.54	13.54	29.05	90.0	90.0	120.0	1556.7
AFX	13.55	13.55	19.35	90.0	90.0	120.0	1557.2
AFY	24.67	12.33	17.20	90.0	90.0	120.0	1408.8
AHT	9.36	9.73	8.50	90.0	90.0	121.3	1809.7
ANA	13.41	13.41	13.41	90.0	90.0	90.0	1985.8
APC	19.33	10.01	8.90	90.0	90.0	90.0	1853.4
APD	19.85	8.35	9.98	90.0	90.0	90.0	1930.1
AST	9.19	9.19	13.48	90.0	90.0	90.0	1750.7
ASV	8.48	8.48	13.83	90.0	90.0	90.0	2006.5
ATN	12.97	12.97	5.17	90.0	90.0	90.0	1835.6
ATO	20.46	20.46	4.96	90.0	90.0	120.0	1996.4
ATS	13.00	21.44	5.17	90.0	90.0	90.0	1661.0
ATT	9.47	15.09	9.23	90.0	90.0	90.0	1814.2
ATV	9.19	14.98	8.29	90.0	90.0	86.5	2104.0
AWO	9.17	14.79	19.08	90.0	90.0	90.0	1851.2
AWW	13.52	13.52	7.61	90.0	90.0	90.0	1721.4
BCT	8.71	8.71	5.01	90.0	90.0	90.0	2101.6
BEA	12.46	12.46	26.22	90.0	90.0	90.0	1567.5
BEC	12.62	12.62	13.02	90.0	90.0	90.0	1540.3
BIK	8.64	4.96	7.36	90.0	115.2	90.0	2095.5
BOF	7.50	12.97	13.32	90.0	90.0	90.0	1850.5
BOG	20.04	23.55	12.62	90.0	90.0	90.0	1608.2
BOZ	14.23	36.22	14.09	90.0	90.0	90.0	1263.6
BPH	12.95	12.95	25.96	90.0	90.0	120.0	1481.0
BRE	6.73	17.07	7.59	90.0	95.3	90.0	1839.0
BSV	17.39	17.39	17.39	90.0	90.0	90.0	1821.0
CAN	12.37	12.37	5.18	90.0	90.0	120.0	1744.0
CAS	16.60	13.78	4.98	90.0	90.0	90.0	2100.0
CDO	7.34	18.21	13.75	90.0	90.0	91.8	1954.5
CFI	13.72	5.19	25.72	90.0	90.2	90.0	1745.0
CGF	15.54	17.15	7.23	90.0	95.5	90.0	1873.4
CGS	8.44	14.10	15.70	90.0	90.0	90.0	1708.3
CHA	9.20	9.20	9.20	94.8	94.8	94.8	1555.6
CON	22.47	13.42	12.35	90.0	69.4	90.0	1602.9
CZP	9.40	9.40	15.24	90.0	90.0	120.0	2054.1
DAC	18.39	7.39	9.89	90.0	109.0	90.0	1884.4
DDR	13.89	13.89	39.92	90.0	90.0	120.0	1794.1

DFO	21.92	21.92	21.03	90.0	90.0	120.0	1505.5
DFT	7.09	7.09	8.64	90.0	90.0	90.0	1835.3
DOH	13.61	13.66	11.13	90.1	90.5	119.8	1888.7
DON	18.86	23.26	8.59	90.0	90.0	90.0	1693.4
EAB	12.99	12.99	14.94	90.0	90.0	120.0	1645.3
EDI	9.51	9.51	6.35	90.0	90.0	90.0	1734.7
EMT	17.13	17.13	27.97	90.0	90.0	120.0	1347.1
EON	14.97	17.98	25.59	90.0	90.0	90.0	1738.6
EPI	8.93	17.41	9.87	90.1	124.0	90.1	1882.7
ERI	12.91	12.91	15.10	90.0	90.0	120.0	1647.0
ESV	9.70	12.30	22.86	90.0	90.0	90.0	1754.8
ETR	20.51	20.51	8.42	90.0	90.0	120.0	1562.4
EUO	13.73	22.52	20.11	90.0	90.0	90.0	1796.9
EZT	10.21	12.47	21.64	90.0	90.0	90.0	1737.4
FAR	12.34	12.34	35.61	90.0	90.0	120.0	1785.7
FAU	24.23	24.23	24.23	90.0	90.0	90.0	1347.4
FER	13.99	7.39	18.58	90.0	90.0	90.0	1869.1
FRA	12.36	12.36	25.40	90.0	90.0	120.0	1781.0
GIS	9.60	9.60	10.13	90.0	90.0	90.0	1710.2
GIU	12.31	12.31	40.75	90.0	90.0	120.0	1789.9
GME	13.56	13.56	9.65	90.0	90.0	120.0	1558.8
GON	16.49	19.94	5.03	90.0	90.0	90.0	1931.4
GOO	8.62	11.55	17.08	90.0	90.0	90.0	1878.1
HEU	17.48	17.55	7.34	90.0	116.4	90.0	1779.7
IFR	18.60	13.42	7.63	90.0	102.0	90.0	1713.3
IHW	13.63	23.97	18.07	90.0	90.0	90.0	1893.1
IMF	14.09	56.89	19.79	90.0	90.0	90.0	1811.7
IRR	19.01	19.01	14.14	90.0	90.0	120.0	1172.1
ISV	12.82	12.82	25.33	90.0	90.0	90.0	1534.2
ITE	20.54	9.71	19.55	90.0	90.0	90.0	1637.7
ITH	12.54	11.44	22.08	90.0	90.0	90.0	1764.7
ITR	11.43	22.08	25.08	90.0	90.0	90.0	1764.6
ITW	10.17	15.04	8.83	90.0	105.2	90.0	1835.8
IWR	20.98	13.44	12.49	90.0	90.0	90.0	1587.0
IWS	26.51	26.51	12.92	90.0	90.0	90.0	1494.0
IWV	27.82	25.25	13.71	90.1	90.0	90.0	1574.1
IWW	41.62	12.81	12.50	89.8	90.0	90.0	1676.1
JBW	7.48	7.84	5.06	90.0	90.0	90.0	2015.1
JOZ	12.81	13.24	13.96	90.0	90.0	90.0	1686.6
JRY	8.09	9.07	17.13	90.0	90.0	90.0	1907.3
JSN	8.64	6.91	15.00	90.0	95.6	90.0	1790.4
JST	15.21	15.21	15.21	90.0	90.0	90.0	1362.3
JSW	15.80	9.72	16.75	90.0	90.0	90.0	1862.0
KFI	18.38	18.38	18.38	90.0	90.0	90.0	1543.4
LAU	14.16	12.99	7.59	90.0	109.8	90.0	1824.0
LEV	12.98	12.98	22.46	90.0	90.0	120.0	1644.5
LIO	12.31	12.31	15.29	90.0	90.0	120.0	1790.0
LOS	12.40	12.40	10.32	90.0	90.0	120.0	1743.4
LOV	7.12	7.12	20.71	90.0	90.0	90.0	1708.9
LTA	11.83	11.83	11.83	90.0	90.0	90.0	1447.3
LTF	30.93	30.93	7.51	90.0	90.0	120.0	1731.4
LTJ	9.19	9.19	9.98	90.0	90.0	90.0	1896.0
LTL	18.01	18.01	7.51	90.0	90.0	120.0	1702.1

LTN	35.53	35.53	35.53	90.0	90.0	90.0	1708.0
MAR	12.42	12.42	30.85	90.0	90.0	120.0	1742.2
MAZ	17.95	17.95	7.51	90.0	90.0	120.0	1714.4
MEI	13.03	13.03	15.59	90.0	90.0	120.0	1478.7
MEL	19.99	19.99	13.45	90.0	90.0	90.0	1781.2
MEP	13.25	13.30	13.23	90.3	90.0	90.3	1969.3
MER	13.99	13.99	9.64	90.0	90.0	90.0	1692.2
MFI	20.07	19.69	13.34	90.0	90.0	90.0	1816.3
MFS	7.46	14.17	18.77	90.0	90.0	90.0	1810.1
MON	7.03	7.03	17.07	90.0	90.0	90.0	1891.5
MOR	18.02	20.04	7.43	90.0	90.0	90.0	1784.7
MOZ	30.96	30.96	7.52	90.0	90.0	120.0	1726.4
MRE	8.32	14.39	20.22	90.0	90.0	90.0	1979.1
MSE	18.29	18.29	20.12	90.0	90.0	90.0	1660.7
MSO	11.73	11.73	11.73	94.1	94.1	94.1	1868.2
MTF	9.43	30.49	7.20	90.0	90.0	90.0	2119.1
MTN	19.63	19.63	19.63	90.0	90.0	90.0	1795.1
MTT	11.16	5.00	21.53	90.0	90.0	90.0	1990.9
MTW	24.93	5.00	24.15	90.0	107.4	90.0	1945.9
MVY	13.94	4.83	8.46	90.0	90.0	90.0	2101.2
MWW	14.17	14.17	24.93	90.0	90.0	120.0	1658.1
NAB	7.16	7.16	12.03	90.0	90.0	90.0	1619.6
NAT	6.37	18.86	9.96	90.0	108.7	90.0	1759.5
NES	14.29	22.08	25.08	90.0	151.6	90.0	1802.9
NON	22.19	15.07	13.59	90.0	90.0	90.0	1931.6
NPO	8.69	8.69	5.19	90.0	90.0	120.0	1763.8
NPT	27.79	27.79	27.79	90.0	90.0	90.0	1339.3
NSI	13.96	4.99	8.54	90.0	105.3	90.0	2087.7
OBW	13.96	13.96	31.12	90.0	90.0	90.0	1250.7
OFF	25.84	25.84	15.09	90.0	90.0	120.0	1646.7
OSI	18.16	18.16	5.07	90.0	90.0	89.3	1908.2
OSO	10.29	10.29	7.67	90.0	90.0	120.0	1276.8
OWE	8.99	14.10	14.23	90.0	90.0	90.0	1768.5
PAU	34.40	34.40	34.40	90.0	90.0	90.0	1646.6
PCR	19.96	13.91	12.19	90.0	114.0	90.0	1936.2
PHI	9.63	14.01	13.96	90.0	90.0	90.0	1696.8
PON	8.90	9.14	16.04	90.0	90.0	90.0	1835.3
PUN	14.56	8.58	19.05	90.0	90.0	90.0	1509.0
RHO	14.77	14.77	14.77	90.0	90.0	90.0	1486.3
RRO	14.66	8.74	17.07	90.0	114.1	90.0	1800.4
RSN	7.08	41.06	7.11	90.0	89.6	90.0	1737.4
RTE	13.96	13.56	7.38	90.0	102.3	90.0	1754.0
RTH	9.71	20.54	9.83	90.0	96.6	90.0	1639.4
RUT	13.21	13.20	12.40	90.0	114.3	90.0	1824.6
RWR	7.68	7.68	26.89	90.0	90.0	90.0	2014.8
RWY	18.47	18.47	18.47	90.0	90.0	90.0	759.7
SAF	14.54	27.62	8.34	90.0	90.0	90.0	1908.3
SAO	13.56	13.56	21.50	90.0	90.0	90.0	1413.3
SAS	14.00	14.00	10.21	90.0	90.0	90.0	1596.6
SAT	12.73	12.73	30.37	90.0	90.0	120.0	1686.8
SAV	18.29	18.29	9.23	90.0	90.0	90.0	1550.6
SBE	18.41	18.41	27.03	90.0	90.0	90.0	1394.1
SBN	12.37	13.66	7.16	90.0	90.0	90.0	1648.2

SBS	17.07	17.07	27.38	90.0	90.0	120.0	1386.7
SBT	17.07	17.07	41.04	90.0	90.0	120.0	1387.4
SFE	11.16	4.99	13.77	90.0	100.6	90.0	1852.9
SFF	11.48	21.70	7.30	90.0	94.8	90.0	1761.8
SFG	25.37	12.43	12.94	90.0	90.0	90.0	1808.0
SFH	5.04	34.07	21.24	90.0	90.0	88.9	1752.2
SFN	5.00	12.78	14.69	102.9	90.5	101.3	1780.7
SFO	22.20	13.57	6.93	90.0	98.4	90.0	1545.3
SFS	14.00	19.87	12.39	90.0	106.5	90.0	1690.9
SFV	19.97	19.97	109.55	90.0	90.0	90.0	1789.8
SGT	10.19	10.19	34.26	90.0	90.0	90.0	1793.4
SIV	9.61	13.98	27.90	90.0	90.0	90.0	1702.5
SOD	8.83	8.83	8.83	90.0	90.0	90.0	1736.9
SOF	20.07	12.21	9.97	90.0	105.6	90.0	1695.2
SOS	20.29	7.26	9.47	90.0	90.0	90.0	1716.4
SSF	16.94	16.94	12.55	90.0	90.0	120.0	1727.8
SSY	22.12	13.76	5.00	90.0	90.0	90.0	1837.2
STF	13.93	18.31	7.40	90.0	99.5	90.0	1713.9
STI	13.42	17.50	17.85	90.0	90.0	90.0	1713.2
STO	29.81	8.42	24.71	90.0	105.3	90.0	1868.8
STW	11.93	11.93	29.56	90.0	90.0	120.0	1642.9
SZR	18.58	14.22	7.46	90.0	90.0	90.0	1823.0
TER	9.64	23.37	19.88	90.0	90.0	90.2	1781.8
THO	13.39	13.41	12.71	90.0	90.0	90.0	1747.4
TOL	12.31	12.31	30.58	90.0	90.0	120.0	1790.0
TON	13.87	17.41	5.00	90.0	90.0	90.0	1982.1
TSC	30.49	30.49	30.49	90.0	90.0	90.0	1352.2
TUN	28.08	19.83	19.39	90.0	92.2	90.0	1775.5
UEI	19.06	9.17	14.81	90.0	90.0	90.0	1850.5
UFI	12.16	12.16	28.04	90.0	90.0	90.0	1540.0
UOS	19.58	7.58	9.00	90.0	90.0	90.0	1794.3
UOZ	8.61	8.61	27.60	90.0	90.0	90.0	1952.3
USI	21.21	12.93	9.58	90.0	108.3	90.0	1600.1
UTL	29.20	13.89	12.31	90.0	105.4	90.0	1575.4
UWY	24.73	12.57	11.50	90.0	90.0	90.6	1674.9
VET	12.99	12.99	4.98	90.0	90.0	90.0	2017.8
VFI	18.29	18.29	8.31	90.0	90.0	120.0	1491.9
VNI	9.93	9.93	33.94	90.0	90.0	90.0	1790.5
VSV	40.96	9.94	10.08	90.0	90.0	90.0	1750.9
WEI	12.00	10.20	10.07	90.0	90.0	90.0	1617.6
YUG	6.57	13.85	9.86	90.0	110.5	90.0	1899.2
ZON	6.92	15.00	17.21	90.0	90.0	90.0	1788.5

Table S3. Structural information of the Zeolitic Imidazolate Frameworks.

ZIF	Lattice constants						Density
	a [Å]	b [Å]	c [Å]	α	β	γ	[kg·m^{-3}]
ABW	27.81	27.81	27.81	94.4	136.3	101.5	770.8
ACO	33.43	33.43	33.43	109.5	109.5	109.5	737.2
AEI	18.24	18.24	36.17	90.0	90.0	94.6	663.3
AEL	23.92	47.21	47.21	139.7	81.0	113.0	860.0
AEN	21.98	21.98	18.65	90.0	90.0	104.9	913.4
AET	34.27	34.35	15.87	90.0	90.0	132.3	863.5
AFG	24.25	24.25	40.46	90.0	90.0	120.0	772.2
AFI	27.43	27.43	16.96	90.0	90.0	120.0	719.7
AFN	18.90	18.90	19.98	77.1	102.9	92.7	781.8
AFO	26.66	26.77	16.24	90.0	90.0	41.3	866.2
AFR	43.09	26.64	27.25	90.0	90.0	90.0	678.0
AFS	25.79	25.79	51.20	90.0	90.0	120.0	629.1
AFT	26.65	26.65	57.16	90.0	90.0	120.0	678.6
AFX	26.47	26.47	37.81	90.0	90.0	120.0	693.0
AFY	24.10	24.10	16.80	90.0	90.0	120.0	627.6
AHT	33.87	33.87	15.43	90.0	90.0	118.1	1019.2
ANA	23.37	23.37	23.37	109.5	109.5	109.5	809.0
APC	20.69	20.69	20.03	90.0	90.0	50.2	804.4
APD	42.38	42.38	19.65	90.0	90.0	45.6	840.7
AST	36.87	37.56	37.55	58.8	60.6	60.6	721.4
ASV	16.39	16.39	26.74	90.0	90.0	90.0	922.1
ATN	38.30	38.30	19.15	94.2	94.2	148.5	750.6
ATO	39.94	39.94	19.36	90.0	90.0	120.0	891.9
ATS	24.40	24.40	20.14	90.0	90.0	62.5	748.2
ATT	19.06	30.37	18.58	90.0	90.0	90.0	739.6
ATV	33.71	33.71	18.51	90.0	90.0	58.4	886.9
AWO	34.23	34.23	37.54	90.0	90.0	63.6	807.5
AWW	27.11	27.11	30.53	90.0	90.0	90.0	708.7
BCT	26.56	26.56	26.56	98.3	98.3	135.3	869.8
BEA	24.28	24.28	51.09	90.0	90.0	90.0	704.1
BEC	24.86	24.86	25.64	90.0	90.0	90.0	669.3
BIK	34.33	34.33	20.09	90.0	90.0	49.9	878.5
BOF	29.55	25.56	26.24	90.0	90.0	90.0	802.7
BOG	32.91	32.91	32.91	106.3	90.3	135.6	698.1
BOZ	38.72	38.72	28.05	90.0	90.0	42.9	532.2
BPH	25.45	25.45	25.45	90.0	90.0	120.0	649.9
BRE	26.77	33.95	30.20	90.0	95.3	90.0	776.3
BSV	30.25	30.25	30.25	109.5	109.5	109.5	746.2
CAN	24.22	24.22	20.30	90.0	90.0	120.0	771.6
CAS	29.21	29.21	32.93	90.7	90.7	39.5	888.9
CDO	38.72	38.71	26.77	90.0	90.0	43.8	859.2
CFI	58.05	28.85	57.75	124.5	160.2	59.3	788.6
CGF	22.57	22.57	28.20	86.3	93.7	84.4	838.3
CGS	16.86	28.16	31.35	90.0	90.0	90.0	712.4
CHA	17.98	17.98	17.98	94.8	94.8	94.8	692.2
CON	25.59	25.59	24.14	107.6	72.4	118.3	712.3
CZP	18.47	18.47	29.96	90.0	90.0	120.0	898.2
DAC	38.95	38.95	19.47	72.9	107.1	136.0	817.2
DDR	30.95	30.95	30.95	51.9	51.9	51.9	780.5

DFO	43.08	43.08	41.33	90.0	90.0	120.0	658.6
DFT	28.34	28.34	17.27	90.0	90.0	90.0	764.6
DOH	27.03	27.11	22.04	90.0	90.0	119.9	804.8
DON	29.42	29.42	16.88	90.0	90.0	78.1	741.9
EAB	25.57	25.57	29.42	90.0	90.0	120.0	715.8
EDI	26.93	26.93	24.89	90.0	90.0	90.0	733.9
EMT	34.32	34.32	56.03	90.0	90.0	120.0	556.5
EON	29.54	35.47	50.50	90.0	90.0	90.0	751.5
EPI	38.57	38.57	20.05	74.6	105.4	55.2	792.7
ERI	25.44	25.44	29.76	90.0	90.0	120.0	715.4
ESV	19.13	24.24	45.06	90.0	90.0	90.0	761.5
ETR	40.76	40.76	16.72	90.0	90.0	120.0	661.1
EUO	25.59	25.80	39.40	90.2	90.3	62.9	801.7
EZT	26.24	26.24	52.49	135.5	124.9	73.3	784.3
FAR	24.49	24.49	70.70	90.0	90.0	120.0	757.9
FAU	34.33	34.33	34.33	60.0	60.0	60.0	556.1
FER	48.10	48.10	24.05	80.2	110.6	144.9	816.5
FRA	24.35	24.35	50.03	90.0	90.0	120.0	773.8
GIS	33.33	33.33	33.33	111.0	111.0	106.5	745.7
GIU	24.14	24.14	79.90	90.0	90.0	120.0	788.6
GME	26.49	26.49	18.86	90.0	90.0	120.0	693.8
GON	25.47	25.47	19.79	90.0	90.0	79.2	841.0
GOO	28.32	28.32	33.56	90.0	90.0	73.5	821.6
HEU	24.16	24.16	28.65	71.7	108.3	89.8	796.3
IFR	22.50	22.50	29.95	80.3	99.7	108.4	753.8
IHW	26.89	26.89	35.24	90.0	90.0	59.3	847.1
IMF	57.20	57.25	38.54	90.0	90.0	27.8	810.7
IRR	38.37	38.37	28.59	90.0	90.0	120.0	472.6
ISV	25.23	25.23	49.85	90.0	90.0	90.0	668.2
ITE	22.35	22.35	38.46	90.0	90.0	129.4	714.1
ITH	24.76	24.56	24.56	54.8	90.0	90.0	761.1
ITR	24.55	24.55	49.53	90.0	90.0	54.7	761.2
ITW	18.12	18.12	17.62	81.4	98.6	69.0	763.3
IWR	24.38	24.38	24.44	90.0	90.0	114.8	703.6
IWS	39.34	39.34	39.34	96.1	96.1	142.0	635.2
IWV	28.13	30.33	36.73	48.2	53.8	77.7	699.9
IWW	82.00	25.24	24.63	89.8	90.0	90.0	728.0
JBW	20.54	29.36	31.85	90.0	90.0	90.0	827.7
JOZ	28.11	25.33	26.56	90.0	90.0	90.0	700.8
JRY	41.32	41.32	41.32	134.7	128.8	70.7	831.0
JSN	16.96	27.14	29.43	90.0	95.6	90.0	786.5
JST	30.04	30.04	30.04	90.0	90.0	90.0	586.8
JSW	30.99	19.06	32.85	90.0	90.0	90.0	819.7
KFI	31.95	31.95	31.95	109.5	109.5	109.5	633.2
LAU	18.86	18.86	29.77	75.6	104.4	95.0	801.4
LEV	20.86	20.86	20.86	75.6	75.6	75.6	715.3
LIO	24.30	24.30	30.18	90.0	90.0	120.0	772.9
LOS	24.74	24.74	20.59	90.0	90.0	120.0	728.7
LOV	27.76	27.76	40.36	90.0	90.0	90.0	767.2
LTA	23.22	23.22	23.22	90.0	90.0	90.0	634.9
LTF	60.65	60.65	29.46	90.0	90.0	120.0	762.7
LTJ	18.33	18.33	19.91	90.0	90.0	90.0	792.4
LTL	35.73	35.73	29.81	90.0	90.0	120.0	723.8

LTN	49.27	49.27	49.27	60.0	60.0	60.0	752.3
MAR	24.31	24.31	60.37	90.0	90.0	120.0	772.5
MAZ	35.27	35.27	29.49	90.0	90.0	120.0	750.9
MEI	25.53	25.53	29.91	90.0	90.0	120.0	667.0
MEL	30.89	30.89	30.89	100.6	100.6	129.1	770.4
MEP	26.36	26.36	26.36	90.0	90.0	90.0	832.3
MER	43.14	43.14	21.57	101.1	101.1	128.1	746.2
MFI	39.43	38.68	26.21	90.0	90.0	90.0	795.7
MFS	24.31	48.62	48.62	144.8	109.9	80.9	785.5
MON	38.80	38.80	39.05	138.4	138.4	59.7	824.4
MOR	26.49	26.49	29.22	90.0	90.0	83.6	780.8
MOZ	60.69	60.69	29.49	90.0	90.0	120.0	761.1
MRE	25.63	51.25	51.25	143.0	113.3	78.8	875.5
MSE	35.88	35.88	39.46	90.0	90.0	90.0	730.6
MSO	23.07	23.07	23.07	94.1	94.1	94.1	816.5
MTF	31.37	31.37	28.31	90.0	90.0	34.4	926.8
MTN	26.68	26.68	26.68	120.0	120.0	90.0	838.6
MTT	19.58	42.19	21.88	90.0	90.0	90.0	879.6
MTW	49.72	49.72	23.96	72.3	107.7	157.2	849.0
MVY	18.97	16.62	27.36	90.0	90.0	90.0	922.1
MWW	27.69	27.69	48.43	90.0	90.0	120.0	742.0
NAB	31.25	31.25	31.25	125.8	125.8	80.1	684.8
NAT	39.76	39.76	19.88	95.9	95.9	142.7	734.2
NES	25.51	32.74	27.82	49.3	76.0	55.6	792.1
NON	19.91	25.34	26.02	45.4	65.6	69.7	859.4
NPO	33.48	33.48	19.99	90.0	90.0	120.0	819.5
NPT	39.14	39.14	39.14	60.0	60.0	60.0	562.7
NSI	55.26	19.73	35.86	90.0	153.0	90.0	895.3
OBW	36.42	36.42	36.42	135.5	135.5	64.8	537.9
OFF	25.45	25.45	29.72	90.0	90.0	120.0	715.6
OSI	52.81	52.81	26.41	92.2	92.2	157.3	762.0
OSO	20.66	20.66	30.77	90.0	90.0	120.0	524.7
OWE	28.01	28.26	17.86	90.0	90.0	90.0	750.0
PCR	68.84	68.84	68.84	90.0	90.0	90.0	682.5
PHI	23.90	23.90	24.22	68.9	111.1	110.5	853.0
PAU	33.74	33.74	27.70	90.0	90.0	69.0	720.4
PON	17.41	17.89	31.38	90.0	90.0	90.0	813.6
PUN	29.22	17.23	38.25	90.0	90.0	90.0	619.5
RHO	25.80	25.80	25.80	109.5	109.5	109.5	601.3
RRO	28.82	17.18	33.57	90.0	114.1	90.0	786.6
RSN	81.96	81.96	27.73	90.0	90.0	19.5	768.3
RTE	19.12	19.12	29.01	81.2	98.8	91.6	768.0
RTH	22.34	22.34	19.34	87.2	92.8	50.6	715.6
RUT	18.32	18.32	24.32	73.0	107.0	90.0	802.2
RWR	57.26	57.26	57.26	149.3	149.3	44.0	869.7
RWY	33.10	33.10	33.10	109.5	109.5	109.5	284.8
SAF	63.52	63.52	31.76	126.5	62.5	150.1	833.7
SAO	28.65	28.65	28.65	123.9	123.9	83.4	596.9
SAS	21.87	21.87	21.87	102.1	102.1	125.5	699.7
SAT	24.61	24.61	24.61	61.2	61.2	61.2	735.5
SAV	36.73	36.73	18.54	90.0	90.0	90.0	635.8
SBE	36.92	36.92	36.92	121.3	121.3	87.8	607.8

SBN	28.15	26.44	28.15	90.0	120.0	90.0	730.6
SBS	34.19	34.19	54.86	90.0	90.0	120.0	572.9
SBT	33.78	33.78	33.78	60.8	60.8	60.8	572.7
SFE	21.92	19.62	27.19	90.7	100.4	90.1	806.8
SFF	22.47	42.49	28.60	90.0	94.8	90.0	779.4
SFG	50.03	24.52	25.52	90.0	90.0	90.0	783.3
SFH	66.95	66.95	41.45	90.0	90.0	17.2	772.4
SFN	50.31	50.31	28.62	76.6	103.4	157.0	772.3
SFO	25.54	25.54	27.22	82.8	97.2	117.1	678.3
SFS	27.54	39.08	24.37	90.0	106.5	90.0	737.9
SFV	36.22	36.22	72.44	148.2	148.2	45.6	804.6
SGT	33.88	33.88	55.70	90.0	90.0	69.0	710.5
SIV	30.68	30.68	30.68	109.5	109.5	109.5	715.5
SOD	23.07	23.07	19.59	76.7	103.3	117.3	742.9
SOF	40.15	28.74	18.74	90.0	90.0	90.0	735.5
SOS	33.29	33.29	24.66	90.0	90.0	120.0	755.8
SSF	19.47	41.89	26.17	90.0	90.0	90.0	869.4
SSY	22.58	22.58	29.06	84.3	95.7	74.5	752.7
STF	24.66	22.03	21.75	68.5	56.3	55.2	741.1
STI	58.60	16.55	48.58	90.0	105.3	90.0	816.6
STO	25.70	42.53	26.98	90.0	102.6	90.0	737.1
STW	23.37	23.37	57.89	90.0	90.0	120.0	726.5
SZR	22.92	22.92	29.22	90.0	90.0	105.1	805.2
TER	24.90	24.90	39.07	90.0	90.0	44.7	777.5
THO	27.16	27.17	25.12	90.0	90.0	90.0	714.9
TOL	24.30	24.30	60.37	90.0	90.0	120.0	772.9
TON	21.85	21.85	19.65	90.0	90.0	77.1	869.7
TSC	42.29	42.29	42.29	60.0	60.0	60.0	594.8
TUN	33.54	33.54	37.85	88.2	91.8	109.6	793.6
UEI	34.50	47.82	41.91	44.6	76.8	58.6	790.3
UFI	32.44	32.44	32.44	136.6	136.6	63.0	666.3
UOS	38.76	30.00	17.81	90.0	90.0	90.0	768.1
UOZ	16.60	16.60	53.24	90.0	90.0	90.0	903.6
USI	24.28	24.28	18.72	74.5	105.5	117.2	711.1
UTL	31.64	31.64	24.09	76.1	103.9	129.2	699.0
UWY	48.85	24.72	22.51	90.0	90.0	90.0	731.5
VET	25.33	25.33	19.44	90.0	90.0	90.0	903.5
VFI	35.07	35.07	15.97	90.0	90.0	120.0	701.3
VNI	19.54	19.54	66.84	90.0	90.0	90.0	778.7
VSV	82.46	82.46	82.52	160.7	160.7	27.3	776.8
WEI	30.86	30.86	19.73	90.0	90.0	99.3	714.8
YUG	33.65	33.65	26.26	77.7	102.3	72.2	803.0
ZON	27.14	29.44	33.77	90.0	90.0	90.0	786.2

Table S4. Pore sizes (Pore Limiting Diameter PLD and Largest Cavity Diameter LCD) and accessible space (Accessible Volume AV and Accessible Surface Area ASA) of the targeted structures calculated using the Zeo++ code [1]. Results on the accessible space correspond to a probe radius of 1.7 Å.

	Zeolites				**ZIFs**			
	Pore sizes		**AV**	**ASA**	**Pore sizes**		**AV**	**ASA**
	PLD [Å]	**LCD [Å]**	**[$cm^3 \cdot g^{-1}$]**	**[$m^2 \cdot g^{-1}$]**	**PLD [Å]**	**LCD [Å]**	**[$cm^3 \cdot g^{-1}$]**	**[$m^2 \cdot g^{-1}$]**
ABW	1.78	2.76	0.0	0.0	6.35	7.66	0.2684	2822.5
ACO	2.89	4.09	0.0	0.0	6.08	8.00	0.3248	2875.3
AEI	3.25	6.77	0.0	0.0	6.80	13.92	0.4813	2707.9
AEL	3.92	5.01	0.0071	265.3	7.58	10.03	0.1704	2072.0
AEN	2.96	3.80	0.0	0.0	6.48	7.71	0.1372	1687.7
AET	7.56	8.36	0.0480	427.3	14.12	15.58	0.2251	1484.7
AFG	1.92	5.74	0.0	0.0	5.18	11.58	0.2890	2635.0
AFI	6.87	7.74	0.0427	489.5	14.22	15.69	0.3812	2733.7
AFN	2.86	4.69	0.0	0.0	6.07	11.01	0.2933	2508.9
AFO	4.21	5.10	0.0094	268.1	8.45	10.28	0.1893	1892.4
AFR	6.34	7.82	0.0628	728.5	12.97	15.60	0.4692	2741.9
AFS	5.58	8.94	0.0751	897.8	12.29	18.26	0.5845	2446.1
AFT	3.13	7.18	0.0	0.0	6.61	14.62	0.4504	2691.1
AFX	3.12	7.19	0.0	0.0	7.62	14.04	0.4374	2626.2
AFY	5.47	7.63	0.0732	1128.3	11.41	15.31	0.6030	2720.0
AHT	2.87	4.23	0.0	0.0	5.04	7.43	0.0977	1482.3
ANA	1.90	3.67	0.0	0.0	6.62	7.85	0.2133	2533.7
APC	2.82	3.50	0.0	0.0	5.34	7.84	0.2361	2687.3
APD	3.14	4.35	0.0	0.0	7.35	8.80	0.1884	2239.1
AST	1.16	6.25	0.0	0.0	5.52	12.42	0.3450	2771.4
ASV	3.78	4.73	0.0040	207.5	7.58	9.37	0.1437	1706.8
ATN	3.62	5.36	0.0079	251.7	8.04	11.05	0.3039	2816.8
ATO	4.91	5.14	0.0109	269.9	9.53	11.04	0.1585	1635.7
ATS	6.13	6.61	0.0461	586.8	12.14	12.75	0.3399	2387.6
ATT	2.97	4.36	0.0	0.0	6.84	10.10	0.3234	2796.8
ATV	1.99	3.65	0.0	0.0	6.75	8.15	0.1242	1935.2
AWO	3.23	4.68	0.0	0.0	6.88	9.35	0.2433	2398.8
AWW	3.58	6.99	0.0246	483.0	8.63	13.97	0.3784	2804.2
BCT	1.70	2.77	0.0	0.0	5.03	7.43	0.1198	2373.4
BEA	5.57	6.14	0.0666	917.0	10.67	12.57	0.4525	2293.3
BEC	6.06	6.34	0.0705	892.0	12.80	13.36	0.5034	2571.5
BIK	2.84	3.44	0.0	0.0	5.90	7.44	0.1353	2232.3
BOF	3.78	4.98	0.0095	394.5	8.63	9.72	0.2377	2219.3
BOG	6.54	7.95	0.0607	764.2	12.98	16.38	0.4480	2349.0
BOZ	4.69	8.57	0.0900	1186.9	10.65	17.86	0.8144	3581.2
BPH	5.58	8.95	0.0763	882.2	11.54	17.97	0.5356	2645.4
BRE	2.70	4.86	0.0	0.0	6.23	10.15	0.2631	2590.0
BSV	3.49	4.85	0.0061	338.3	8.07	10.27	0.3152	2631.2
CAN	5.46	5.71	0.0147	329.5	10.71	11.67	0.2839	2492.1
CAS	2.28	3.86	0.0	0.0	5.51	8.04	0.1359	2026.4
CDO	2.71	4.87	0.0	0.0	6.43	10.00	0.1835	1826.0
CFI	6.71	6.78	0.0400	457.6	13.11	13.64	0.2705	2166.6
CGF	2.89	5.20	0.0	0.0	6.44	10.39	0.2106	2095.1

CGS	3.62	5.28	0.0143	481.4	8.34	11.83	0.3842	2609.5
CHA	3.15	6.70	0.0	0.0	6.38	13.34	0.4438	2575.9
CON	4.94	7.07	0.0573	819.8	10.28	13.93	0.4336	2278.5
CZP	3.40	3.78	0.0	0.0	6.58	8.47	0.1651	1691.2
DAC	3.11	4.56	0.0	0.0	6.60	9.47	0.2287	2277.5
DDR	3.17	7.05	0.0	0.0	6.51	13.85	0.2716	2141.3
DFO	6.73	10.95	0.0819	880.6	13.89	21.74	0.5337	2405.8
DFT	3.24	4.58	0.0	0.0	6.97	9.21	0.2636	2892.3
DOH	1.57	6.63	0.0	0.0	4.64	15.12	0.2581	2160.4
DON	7.73	8.27	0.0583	514.1	15.57	16.57	0.3559	2420.9
EAB	2.89	6.59	0.0	0.0	6.43	12.91	0.3972	2523.0
EDI	2.26	4.85	0.0	0.0	6.84	9.32	0.3478	2900.0
EMT	6.76	10.93	0.1360	999.6	14.10	22.83	0.7883	2615.2
EON	6.28	7.25	0.0257	318.6	12.55	14.60	0.3200	2420.6
EPI	3.12	4.93	0.0	0.0	6.78	10.30	0.2512	2177.5
ERI	2.78	6.50	0.0	0.0	6.20	13.06	0.3894	2675.5
ESV	3.30	6.05	0.0	0.0	7.34	11.98	0.3202	2423.2
ETR	8.83	9.55	0.0613	463.4	19.10	19.92	0.5119	2486.4
EUO	4.44	6.37	0.0267	477.0	9.02	12.45	0.2680	1951.0
EZT	5.54	6.06	0.0324	561.2	10.89	11.94	0.2953	2264.4
FAR	1.61	5.72	0.0	0.0	3.67	13.37	0.3220	2259.5
FAU	6.76	10.59	0.1358	1004.1	14.14	22.39	0.7914	2616.8
FER	4.13	5.34	0.0046	203.5	8.80	10.36	0.2285	2098.8
FRA	1.64	5.72	0.0	0.0	3.53	13.22	0.3100	2147.4
GIS	2.51	4.37	0.0	0.0	5.28	8.77	0.2993	2847.8
GIU	1.58	5.71	0.0	0.0	3.51	13.41	0.2541	1637.0
GME	6.41	7.20	0.0426	559.3	12.44	13.82	0.4371	2763.4
GON	5.06	5.88	0.0172	317.9	9.66	11.87	0.1988	2014.7
GOO	2.47	3.61	0.0	0.0	5.92	8.00	0.2196	2434.9
HEU	3.28	5.52	0.0	0.0	6.67	10.80	0.2528	2293.2
IFR	5.88	6.73	0.0444	643.7	12.05	13.11	0.3334	2124.3
IHW	3.09	6.12	0.0	0.0	6.56	12.40	0.2127	1721.9
IMF	4.69	6.87	0.0239	521.6	9.41	13.74	0.2619	1874.9
IRR	11.77	14.07	0.2426	1279.6	24.09	28.87	1.1109	2764.7
ISV	5.82	6.48	0.0712	888.3	11.70	12.88	0.4960	2563.3
ITE	3.54	7.60	0.0442	634.1	7.08	15.11	0.3912	2582.1
ITH	4.70	6.25	0.0217	504.6	9.77	13.00	0.3152	2260.9
ITR	4.68	6.01	0.0227	525.8	9.47	12.37	0.3148	2269.6
ITW	3.03	4.16	0.0	0.0	7.35	9.14	0.2861	2763.2
IWR	5.16	7.20	0.0595	828.8	10.57	14.77	0.4493	2314.0
IWS	6.30	7.91	0.0889	963.3	13.30	15.89	0.5632	2591.7
IWV	6.28	8.11	0.0828	798.7	13.19	16.31	0.4490	2020.7
IWW	5.63	6.23	0.0398	654.7	11.21	13.23	0.3853	2348.0
JBW	2.79	3.41	0.0	0.0	6.60	8.12	0.1852	2622.5
JOZ	2.52	4.39	0.0	0.0	6.80	9.46	0.3835	3208.2
JRY	3.88	4.06	0.0029	211.6	7.40	8.65	0.2082	2227.3
JSN	3.07	4.69	0.0	0.0	6.16	9.51	0.2651	2500.6
JST	3.51	5.09	0.0249	1164.2	7.92	11.84	0.6446	3469.7
JSW	2.13	4.68	0.0	0.0	4.74	9.76	0.2338	2362.0
KFI	3.50	10.12	0.0489	670.6	7.85	21.66	0.5364	2846.6
LAU	3.30	5.17	0.0	0.0	7.34	10.59	0.2532	2380.5
LEV	2.86	6.57	0.0	0.0	6.36	12.44	0.3818	2748.0
LIO	1.55	5.70	0.0	0.0	3.66	13.43	0.3098	2148.0

LOS	2.03	5.74	0.0	0.0	5.98	11.56	0.3521	2872.0
LOV	3.14	4.63	0.0	0.0	6.81	8.28	0.2759	2777.9
LTA	3.58	10.50	0.0830	797.4	7.87	19.75	0.5559	2856.9
LTF	6.88	7.57	0.0186	249.2	13.85	15.15	0.3066	2527.2
LTJ	2.64	3.75	0.0	0.0	6.05	8.27	0.2296	2621.9
LTL	6.98	9.48	0.0550	510.8	14.25	19.63	0.3730	2473.4
LTN	1.73	9.64	0.0	0.0	3.69	19.97	0.3009	1929.5
MAR	2.03	5.80	0.0	0.0	4.75	11.28	0.2730	2620.1
MAZ	6.91	7.60	0.0264	289.7	13.83	15.19	0.3250	2433.5
MEI	6.32	7.63	0.0739	907.1	12.48	14.90	0.5068	2430.3
MEL	4.83	6.68	0.0272	547.2	9.74	14.07	0.3034	2302.6
MEP	1.09	4.74	0.0	0.0	3.73	9.82	0.1863	2148.6
MER	3.60	5.82	0.0093	287.0	8.07	11.85	0.3332	2606.9
MFI	4.69	6.47	0.0234	504.6	9.50	12.75	0.2698	2068.6
MFS	4.79	6.29	0.0208	416.7	9.77	12.18	0.2718	2373.4
MON	2.82	3.29	0.0	0.0	5.86	7.47	0.1940	2506.3
MOR	5.68	6.15	0.0237	357.8	11.29	12.10	0.2776	2155.0
MOZ	6.97	9.48	0.0273	313.2	14.26	19.29	0.3149	2445.8
MRE	5.02	5.97	0.0113	259.1	9.99	11.36	0.1598	1893.8
MSE	5.92	6.65	0.0464	713.1	11.57	12.82	0.3920	2410.1
MSO	1.58	6.00	0.0	0.0	3.94	12.80	0.2407	2144.7
MTF	3.44	5.59	0.0089	221.4	4.93	7.91	0.0994	1689.3
MTN	2.08	6.81	0.0	0.0	4.19	11.87	0.2097	2109.3
MTT	4.36	5.40	0.0095	268.8	9.40	10.78	0.1559	1658.3
MTW	5.11	5.74	0.0184	337.0	10.55	11.23	0.2014	1871.0
MVY	2.59	3.02	0.0	0.0	6.26	7.14	0.1149	1930.7
MWW	4.30	9.07	0.0467	717.2	8.85	17.95	0.3694	2290.3
NAB	2.71	3.87	0.0	0.0	6.98	8.40	0.4018	3289.0
NAT	2.83	3.72	0.0	0.0	6.78	7.73	0.3206	3032.5
NES	4.36	5.57	0.0273	551.6	9.62	12.30	0.2858	1826.7
NON	1.67	5.91	0.0	0.0	3.61	11.66	0.1941	1866.0
NPO	4.06	4.22	0.0025	216.7	7.75	8.55	0.2000	2594.5
NPT	3.17	9.85	0.0	0.0	6.83	20.44	0.7237	3452.1
NSI	2.46	3.19	0.0	0.0	5.77	7.25	0.1180	1956.2
OBW	4.84	8.91	0.0865	980.3	10.11	18.59	0.8094	3444.9
OFF	6.00	6.53	0.0264	427.2	11.48	13.50	0.3822	2708.0
OSI	5.74	6.00	0.0195	329.3	12.20	12.73	0.2961	2642.5
OSO	5.67	5.88	0.0788	1278.4	12.17	12.64	0.8357	3685.4
OWE	3.26	5.27	0.0	0.0	7.39	10.68	0.3120	2675.2
PCR	3.41	5.25	0.0042	166.9	6.86	10.63	0.1936	1975.7
PHI	3.19	4.88	0.0	0.0	7.17	10.60	0.3526	2779.0
PON	3.44	4.47	0.0054	295.9	8.12	9.53	0.2423	2353.6
PUN	3.86	5.02	0.0235	857.8	8.97	10.99	0.5680	3161.0
RHO	3.49	9.84	0.0721	765.1	8.28	20.42	0.6268	2957.0
RRO	3.37	4.11	0.0018	237.4	7.45	8.62	0.2622	2533.0
RSN	2.97	4.19	0.0	0.0	6.74	8.47	0.2798	2733.3
RTE	3.45	6.41	0.0217	456.8	7.33	12.49	0.2924	2507.7
RTH	3.52	7.49	0.0438	641.1	7.40	14.99	0.3871	2599.5
RUT	1.61	5.48	0.0	0.0	4.67	10.91	0.2482	2298.9
RWR	2.72	3.95	0.0	0.0	6.55	8.77	0.1648	2180.3
RWY	6.31	15.35	0.4995	2549.9	14.74	32.88	2.4295	4177.1
SAF	5.78	6.44	0.0264	336.2	11.18	12.82	0.2149	1961.3
SAO	6.17	7.93	0.1061	1093.9	12.87	17.13	0.6737	2124.9

SAS	3.57	8.26	0.0521	668.5	7.22	16.48	0.4292	2549.1
SAT	2.60	6.30	0.0	0.0	5.94	13.64	0.3667	2369.3
SAV	3.49	8.05	0.0361	495.7	7.69	17.24	0.5264	2839.5
SBE	6.78	12.05	0.1228	835.8	13.68	23.59	0.6505	2638.6
SBN	3.38	4.53	0.0	0.0	7.08	8.80	0.3472	2937.6
SBS	6.74	10.92	0.1263	999.9	13.90	22.66	0.7304	2705.9
SBT	6.73	10.61	0.1272	1016.1	14.14	22.19	0.7355	2679.6
SFE	5.52	5.90	0.0300	444.9	11.31	12.30	0.2507	1916.7
SFF	5.06	7.35	0.0395	561.9	10.26	14.54	0.3107	2022.7
SFG	4.99	6.38	0.0252	450.5	9.97	13.00	0.2848	2280.5
SFH	6.36	7.36	0.0492	516.7	13.13	14.57	0.3095	2017.5
SFN	6.07	7.28	0.0473	498.2	12.45	14.34	0.3129	2036.2
SFO	6.50	7.46	0.0637	750.4	12.79	15.16	0.4668	2702.3
SFS	5.40	7.09	0.0452	680.4	10.72	14.40	0.3641	2317.3
SFV	5.04	6.92	0.0279	547.4	4.49	13.83	0.2457	2140.4
SGT	1.59	7.27	0.0	0.0	7.44	10.73	0.3631	2891.3
SIV	3.16	4.85	0.0	0.0	5.66	11.90	0.3431	3138.9
SOD	2.01	5.70	0.0	0.0	7.85	10.33	0.3559	2548.4
SOF	3.45	4.62	0.0109	493.3	7.88	9.25	0.3571	2831.1
SOS	3.52	4.15	0.0018	168.9	11.22	15.04	0.3394	1923.1
SSF	5.57	6.94	0.0463	566.7	10.40	12.53	0.2081	1552.2
SSY	5.30	6.65	0.0315	467.0	10.53	15.11	0.3437	2215.9
STF	5.21	7.56	0.0441	630.4	8.99	12.47	0.3823	2356.7
STI	4.39	5.68	0.0229	574.4	11.24	13.19	0.2501	2050.5
STO	5.58	6.47	0.0263	381.7	7.17	13.81	0.3707	2349.9
STW	4.34	5.09	0.0241	697.6	8.74	10.39	0.3707	2583.1
SZR	4.04	5.76	0.0136	347.3	8.40	11.04	0.2404	2273.5
TER	4.51	6.32	0.0224	547.9	8.92	12.55	0.2931	2325.1
THO	2.69	4.62	0.0	0.0	7.18	9.12	0.3820	2995.0
TOL	1.55	5.70	0.0	0.0	3.60	13.35	0.3076	2143.3
TON	4.60	5.04	0.0101	294.1	9.60	9.86	0.1678	1838.4
TSC	3.61	15.65	0.1379	820.3	7.84	31.46	0.6515	2340.2
TUN	5.02	8.04	0.0312	562.4	9.97	15.76	0.2851	1903.5
UEI	3.19	4.98	0.0	0.0	6.94	10.66	0.2478	2500.8
UFI	3.24	9.59	0.0	0.0	7.26	18.58	0.4764	2496.1
UOS	3.54	5.28	0.0081	397.9	7.69	10.55	0.2861	2589.1
UOZ	0.70	4.99	0.0	0.0	4.34	9.46	0.1517	1914.0
USI	5.84	6.31	0.0504	851.8	11.50	12.93	0.4259	2255.6
UTL	6.86	8.95	0.0828	812.1	13.62	17.75	0.4509	1943.0
UWY	5.68	8.10	0.0411	672.5	12.17	16.31	0.3753	2389.2
VET	5.59	5.76	0.0169	312.4	11.15	11.68	0.1542	1358.3
VFI	11.23	11.75	0.1309	715.3	21.09	22.22	0.4747	1965.2
VNI	2.42	4.27	0.0	0.0	5.86	8.91	0.2630	2711.3
VSV	2.91	3.71	0.0	0.0	6.48	8.72	0.2656	2720.7
WEI	3.07	3.83	0.0	0.0	6.24	8.80	0.3664	3092.8
YUG	2.43	3.54	0.0	0.0	5.46	8.25	0.2347	2573.9
ZON	3.03	5.50	0.0	0.0	6.36	10.80	0.2729	2525.8

Table S5. Heat of adsorption of the targeted gas molecules in the set of zeolites and their respective Zeolitic Imidazolate Frameworks.

	Ar		O_2		CO_2		N_2		CH_4	
	Zeo	**ZIF**	**Zeo**	**ZIF**	**Zeo**	**ZIF**	**Zeo**	**ZIF**	**Zeo**	**ZIF**
ABW	0	10.02	0	10.45	0	20.85	0	10.31	0	13.04
ACO	0	10.31	0	10.03	0	20.74	0	8.99	0	13.59
AEI	0	9.08	0	9.47	0	20.92	0	9.32	0	12.28
AEL	14.69	13.25	16.42	13.97	28.85	30.21	13.94	13.94	21.21	17.87
AEN	0	11.97	0	12.75	0	32.18	0	12.16	0	15.30
AET	9.47	13.53	10.19	14.76	16.53	38.94	8.87	14.41	12.83	17.57
AFG	0	10.38	0	10.91	0	24.37	0	10.89	0	13.64
AFI	10.75	11.65	11.76	12.31	19.70	30.73	10.14	12.27	15.01	15.68
AFN	0	11.26	0	11.97	0	33.37	0	11.82	0	14.93
AFO	14.41	12.82	16.18	13.57	28.73	28.40	13.70	13.36	21.07	17.29
AFR	11.11	11.21	11.92	11.76	20.24	28.12	10.31	11.57	15.21	16.49
AFS	10.36	9.52	11.31	9.96	20.87	22.91	10.05	9.46	14.41	12.78
AFT	0	9.32	0	9.75	0	23.40	0	9.65	0	12.60
AFX	0	9.42	0	9.84	0	22.41	0	9.76	0	12.71
AFY	11.98	8.55	12.43	8.68	20.44	21.36	10.96	8.31	14.75	11.05
AHT	0	13.53	0	14.39	0	41.65	0	14.36	0	17.39
ANA	0	9.54	0	9.90	0	17.32	0	9.75	0	12.20
APC	0	10.60	0	11.12	0	25.16	0	11.17	0	13.87
APD	0	12.08	0	12.82	0	30.56	0	12.88	0	16.73
AST	0	12.34	0	12.72	0	21.88	0	11.89	0	20.12
ASV	15.62	14.17	17.50	15.34	28.67	33.69	14.88	14.66	0	19.13
ATN	15.41	10.06	17.57	10.53	32.27	22.00	15.12	10.26	0	12.99
ATO	13.98	12.40	15.84	13.14	27.42	28.85	13.32	13.22	20.96	16.59
ATS	11.04	10.75	12.07	11.39	20.94	25.30	10.61	11.28	15.33	14.56
ATT	0	9.75	0	10.18	0	21.10	0	9.89	0	12.83
ATV	0	12.80	0	13.62	0	35.83	0	13.70	0	17.69
AWO	0	10.51	0	11.00	0	24.90	0	10.86	0	13.84
AWW	13.50	9.99	15.07	10.49	26.28	24.12	0	10.40	0	13.42
BCT	0	10.82	0	11.41	0	20.35	0	10.88	0	13.55
BEA	10.98	12.70	12.20	13.37	21.32	35.20	10.42	13.02	15.90	17.75
BEC	10.79	11.50	12.01	12.03	21.40	26.64	10.23	11.46	15.77	15.73
BIK	0	12.37	0	12.99	0	25.89	0	12.75	0	16.17
BOF	15.01	11.58	16.91	12.24	28.96	24.41	14.36	11.75	0	16.02
BOG	11.63	11.58	12.89	12.17	22.39	26.95	10.98	11.43	16.92	15.66
BOZ	9.79	7.47	10.68	7.81	18.07	21.11	9.27	7.56	13.59	9.72
BPH	10.93	10.75	11.97	11.40	21.41	28.14	10.31	10.77	15.57	14.97
BRE	0	11.65	0	12.10	0	24.27	0	11.38	0	15.98
BSV	15.13	9.28	16.82	9.95	26.98	22.43	0	9.45	0	11.78
CAN	12.96	10.21	14.64	10.80	25.26	23.23	12.34	10.66	19.31	13.27
CAS	0	12.58	0	13.29	0	29.13	0	12.83	0	16.42
CDO	0	13.27	0	14.09	0	32.06	0	13.60	0	18.01
CFI	10.95	11.70	11.50	12.37	19.16	27.41	10.08	12.00	14.60	15.59
CGF	0	10.41	0	11.10	0	31.62	0	10.27	0	12.99
CGS	13.55	9.86	15.16	10.27	27.02	20.65	12.93	9.98	0	13.52
CHA	0	9.73	0	10.18	0	23.49	0	10.16	0	13.51
CON	11.42	11.17	12.63	11.90	21.72	29.76	10.82	11.10	16.32	14.73
CZP	0	10.27	0	10.69	0	24.17	0	10.14	0	12.79

DAC	0	11.98	0	12.69	0	28.29	0	12.09	0	15.54
DDR	0	10.66	0	11.28	0	25.65	0	10.71	0	13.47
DFO	11.07	10.02	12.25	10.82	21.48	32.41	10.42	10.18	16.19	13.75
DFT	0	10.94	0	11.50	0	34.58	0	11.91	0	15.13
DOH	0	10.75	0	11.35	0	25.90	0	11.03	0	14.14
DON	9.64	12.12	10.42	12.77	16.96	27.36	9.01	12.84	13.16	16.47
EAB	0	9.50	0	9.93	0	24.19	0	9.80	0	13.20
EDI	0	9.00	0	9.59	0	35.22	0	9.61	0	11.38
EMT	8.80	8.54	9.53	8.91	16.30	20.05	8.31	8.65	12.08	11.86
EON	10.99	11.22	12.03	11.81	20.44	29.24	10.43	11.38	15.47	14.98
EPI	0	10.57	0	11.32	0	32.26	0	10.69	0	13.25
ERI	0	10.19	0	10.75	0	25.84	0	10.58	0	13.63
ESV	0	9.82	0	10.34	0	21.47	0	10.04	0	12.66
ETR	10.28	10.05	10.54	10.45	17.49	22.98	9.26	9.95	13.14	13.58
EUO	12.87	12.03	14.19	12.74	25.23	28.04	12.09	12.26	18.57	16.13
EZT	12.47	11.62	13.90	12.30	24.14	26.25	11.81	11.91	18.27	15.67
FAR	0	9.35	0	9.76	0	20.40	0	9.58	0	12.09
FAU	8.59	8.57	9.24	8.95	15.11	19.78	8.11	8.68	11.49	11.96
FER	15.14	12.87	16.97	13.56	29.00	31.27	14.36	13.03	21.72	17.69
FRA	0	9.27	0	9.66	0	19.26	0	9.49	0	11.86
GIS	0	9.42	0	9.81	0	22.11	0	9.86	0	12.22
GIU	0	9.97	0	10.44	0	21.84	0	10.29	0	13.02
GME	10.46	9.98	11.41	10.56	19.04	24.86	9.88	10.13	14.52	13.05
GON	12.75	12.40	14.10	13.17	24.00	26.93	12.03	12.86	18.35	16.41
GOO	0	10.73	0	11.44	0	30.37	0	11.16	0	13.49
HEU	0	12.55	0	13.48	0	32.33	0	12.91	0	16.40
IFR	12.15	11.95	13.40	12.77	23.04	33.82	11.44	12.38	17.37	16.59
IHW	0	12.96	0	13.86	0	32.84	0	13.15	0	17.51
IMF	13.44	12.30	15.09	13.13	26.19	30.51	12.78	12.42	19.82	16.33
IRR	8.54	10.16	9.37	10.88	17.18	26.38	7.91	10.08	12.66	15.30
ISV	10.62	10.96	11.77	11.51	20.71	27.66	10.07	11.04	15.32	15.26
ITE	12.37	10.90	13.56	11.50	23.10	27.22	0	11.20	0	15.15
ITH	13.64	11.21	14.88	11.94	25.32	27.73	12.72	11.41	19.04	14.82
ITR	13.63	11.25	14.85	11.99	25.20	27.73	12.71	11.44	18.97	14.86
ITW	0	11.23	0	11.49	0	24.51	0	10.90	0	15.64
IWR	11.45	11.30	12.68	12.16	22.09	30.46	10.85	11.61	16.46	15.32
IWS	10.11	10.94	11.14	11.54	19.69	28.93	9.55	10.94	14.50	15.15
IWV	10.04	11.80	10.75	12.61	17.83	29.56	9.34	11.84	13.56	16.49
IWW	11.89	11.30	13.27	12.00	23.29	28.05	11.30	11.47	17.33	15.52
JBW	0	11.00	0	11.59	0	29.88	0	11.54	0	14.06
JOZ	0	9.06	0	9.52	0	24.72	0	9.25	0	11.37
JRY	16.46	11.78	18.01	12.55	31.13	29.96	15.49	12.20	0	15.72
JSN	0	11.82	0	12.45	0	29.31	0	12.22	0	16.69
JST	12.15	7.85	13.46	8.17	23.17	17.77	11.58	7.85	0	10.08
JSW	0	11.42	0	12.09	0	30.24	0	12.10	0	15.29
KFI	12.21	8.74	13.35	9.08	25.72	18.49	0	8.83	0	11.74
LAU	0	11.95	0	12.64	0	26.86	0	12.24	0	16.40
LEV	0	9.75	0	10.21	0	22.12	0	10.06	0	12.91
LIO	0	9.73	0	10.17	0	21.37	0	10.02	0	12.71
LOS	0	9.90	0	10.35	0	22.57	0	10.17	0	12.87
LOV	0	10.08	0	10.57	0	29.06	0	10.56	0	13.25
LTA	10.36	11.03	11.25	11.25	18.48	25.43	0	9.94	0	15.15
LTF	11.22	11.07	12.16	11.76	20.83	31.69	10.55	11.45	15.71	14.35

LTJ	0	10.42	0	11.16	0	28.81	0	10.61	0	12.86
LTL	10.96	10.89	11.84	11.51	21.54	31.68	10.24	11.49	15.12	14.41
LTN	0	9.98	0	10.43	0	22.04	0	10.28	0	13.56
MAR	0	10.28	0	10.81	0	24.82	0	10.79	0	13.56
MAZ	10.45	10.87	11.44	11.51	19.32	27.85	9.91	10.81	14.64	14.06
MEI	11.45	10.72	12.38	11.18	21.21	30.46	10.69	10.95	15.58	17.13
MEL	13.23	12.72	14.87	13.45	25.97	28.58	12.63	13.18	19.57	17.26
MEP	0	11.13	0	11.94	0	31.77	0	11.41	0	14.23
MER	15.40	9.08	16.64	9.50	25.40	19.17	14.66	9.32	0	11.60
MFI	13.63	12.67	15.29	13.53	26.56	29.77	12.97	12.94	20.02	17.61
MFS	13.14	12.36	14.60	13.06	25.27	29.40	12.45	12.83	19.00	16.89
MON	0	11.05	0	11.73	0	28.45	0	10.85	0	13.03
MOR	11.72	11.45	12.87	12.21	22.01	31.08	11.05	11.68	16.63	14.80
MOZ	11.14	11.02	12.26	11.66	21.59	30.47	10.50	11.47	15.90	14.45
MRE	13.82	12.60	15.62	13.27	27.33	27.31	13.17	13.12	20.63	16.86
MSE	11.49	12.08	12.80	12.70	22.40	27.84	10.95	12.46	16.67	16.55
MSO	0	12.16	0	12.86	0	26.62	0	12.73	0	16.36
MTF	14.84	12.51	16.41	13.19	29.11	36.60	0	13.15	0	16.43
MTN	0	10.99	0	11.61	0	24.82	0	11.22	0	14.20
MTT	14.32	13.38	16.11	14.24	28.57	35.95	13.68	14.06	21.08	17.66
MTW	12.62	12.66	14.03	13.37	24.15	29.12	11.96	12.95	18.36	16.49
MVY	0	14.24	0	15.24	0	32.95	0	15.14	0	19.15
MWW	13.07	12.33	14.61	13.15	26.58	31.52	12.33	12.80	19.36	17.04
NAB	0	8.26	0	8.62	0	18.36	0	8.40	0	10.27
NAT	0	8.95	0	9.35	0	19.44	0	9.12	0	11.34
NES	12.06	11.83	13.38	12.66	23.68	33.00	11.86	12.12	17.13	15.90
NON	0	12.10	0	12.75	0	26.39	0	12.43	0	16.17
NPO	15.18	11.79	16.60	12.50	28.18	32.56	14.19	13.04	0	15.93
NPT	0	7.76	0	8.16	0	22.95	0	7.88	0	9.89
NSI	0	11.69	0	12.23	0	24.62	0	11.61	0	14.80
OBW	9.21	7.43	9.96	7.75	16.24	21.60	8.72	7.53	12.50	9.41
OFF	11.37	10.59	12.68	11.20	21.82	26.04	10.82	10.87	16.50	14.09
OSI	12.01	11.04	13.33	11.53	22.92	23.52	11.38	11.35	17.38	14.58
OSO	10.17	7.68	11.07	8.06	18.45	18.36	9.65	7.78	13.92	9.85
OWE	0	11.92	0	12.78	0	32.95	0	13.06	0	16.85
PCR	15.52	12.34	17.38	13.12	28.93	28.01	0	12.48	0	16.11
PHI	0	8.93	0	9.28	0	18.63	0	9.10	0	11.43
PON	15.24	11.17	16.98	11.96	28.87	32.32	14.57	11.78	0	14.93
PUN	12.70	8.38	14.14	8.72	24.26	19.04	12.15	8.43	18.01	11.01
RHO	13.96	8.28	13.86	8.62	18.51	17.19	0	8.30	0	10.79
RRO	14.96	12.64	16.33	13.30	26.75	29.13	0	12.63	0	17.25
RSN	0	10.13	0	10.63	0	29.13	0	10.38	0	13.32
RTE	13.77	11.13	15.31	11.79	27.05	29.43	0	11.23	0	14.08
RTH	12.37	10.93	13.49	11.56	23.08	28.18	0	11.22	0	15.05
RUT	0	10.42	0	11.00	0	23.80	0	10.49	0	13.26
RWR	0	12.15	0	12.88	0	28.09	0	12.83	0	16.42
RWY	6.68	5.93	7.12	6.36	11.34	25.37	6.29	6.15	8.76	7.78
SAF	11.34	13.10	12.47	13.90	21.06	29.61	10.69	13.78	16.12	17.70
SAO	9.63	9.21	10.54	9.76	17.78	22.98	9.12	9.42	13.41	12.92
SAS	11.83	10.01	13.02	10.52	22.09	25.17	0	10.37	0	13.60
SAT	0	10.40	0	10.86	0	23.37	0	10.75	0	14.23
SAV	11.43	8.69	12.49	9.03	21.20	18.33	0	8.76	0	11.67
SBE	11.99	9.45	12.88	10.00	21.57	24.40	8.35	9.56	12.15	12.57

SBN	0	8.60	0	8.94	0	18.41	0	8.73	0	10.79
SBS	9.76	9.89	10.07	10.48	17.02	24.60	8.77	9.89	12.90	13.72
SBT	9.74	9.82	10.08	10.39	17.05	24.54	8.79	9.78	12.91	13.57
SFE	11.70	12.30	12.79	13.20	21.89	32.56	11.07	12.53	16.40	16.08
SFF	12.25	11.90	13.37	12.72	22.79	31.35	11.51	12.39	17.13	16.59
SFG	12.48	12.21	13.93	12.89	24.53	27.93	11.85	12.69	18.21	16.56
SFH	10.43	11.79	11.32	12.54	19.07	31.14	9.83	12.17	14.39	15.95
SFN	10.48	11.79	11.38	12.48	19.01	29.57	9.87	12.38	14.45	15.92
SFO	11.11	11.18	11.95	11.75	20.33	30.02	10.33	11.70	15.26	16.34
SFS	12.38	12.44	13.79	13.27	24.56	29.99	11.68	12.76	18.31	16.99
SFV	13.22	11.93	14.86	12.94	26.00	32.21	12.60	12.79	19.58	15.94
SGT	0	8.87	0	9.19	0	18.25	0	8.99	0	11.40
SIV	0	9.22	0	9.62	0	19.03	0	9.35	0	11.99
SOD	0	10.51	0	11.21	0	27.38	0	10.62	0	13.79
SOF	13.43	10.28	14.36	11.15	24.25	37.12	12.44	10.79	0	13.45
SOS	12.86	12.06	14.27	12.74	21.37	30.29	0	12.58	0	16.81
SSF	10.81	12.67	11.92	13.79	20.16	46.68	10.24	15.88	15.40	17.19
SSY	11.64	11.64	12.73	12.30	21.83	29.27	11.01	11.79	16.31	15.79
STF	12.23	11.19	13.33	11.90	22.81	35.10	11.50	11.94	17.01	16.21
STI	13.19	12.56	14.79	13.24	26.18	27.81	12.62	13.10	19.20	17.01
STO	11.69	11.21	12.90	11.87	21.78	27.36	11.01	11.41	16.70	15.49
STW	13.55	10.30	15.00	10.94	26.44	31.74	12.92	10.38	18.96	13.22
SZR	13.38	11.41	14.98	11.97	25.70	26.20	12.79	11.57	19.39	15.01
TER	13.69	12.42	15.24	13.24	25.94	29.64	13.02	13.09	19.53	17.22
THO	0	9.07	0	9.68	0	25.60	0	9.34	0	11.49
TOL	0	9.73	0	10.16	0	21.31	0	10.02	0	12.71
TON	14.58	13.18	16.37	13.92	28.68	29.86	13.88	13.79	21.35	17.67
TSC	8.99	9.43	9.67	9.96	16.45	28.51	9.04	9.91	0	13.83
TUN	13.04	12.56	14.60	13.45	25.99	31.43	12.37	12.56	19.27	16.84
UEI	0	10.16	0	10.58	0	23.09	0	10.38	0	13.39
UFI	0	9.94	0	10.35	0	27.95	0	9.87	0	14.39
UOS	14.49	10.95	16.09	11.37	27.22	24.51	0	10.99	0	14.77
UOZ	0	13.13	0	13.89	0	34.60	0	12.96	0	16.26
USI	11.67	12.18	12.73	13.20	22.65	38.92	10.98	12.42	16.06	17.98
UTL	10.42	12.31	11.43	13.18	19.74	32.00	9.73	12.58	15.19	17.12
UWY	13.15	11.65	14.57	12.41	25.10	29.13	12.24	11.96	18.36	16.01
VET	12.10	13.22	13.42	14.19	23.24	32.14	11.49	13.81	17.51	17.51
VFI	8.01	12.19	8.47	13.20	13.44	38.21	7.42	13.43	10.52	16.91
VNI	0	9.96	0	10.47	0	25.04	0	9.94	0	12.21
VSV	0	9.61	0	10.08	0	21.72	0	9.57	0	12.08
WEI	0	9.20	0	9.79	0	35.46	0	9.89	0	12.16
YUG	0	11.12	0	11.77	0	26.94	0	11.42	0	14.07
ZON	0	11.98	0	12.71	0	30.01	0	12.65	0	17.31

Table S6. Henry coefficients of the targeted gas molecules in the set of zeolites.

	Zeolites				
	Ar	**O_2**	**CO_2**	**N_2**	**CH_4**
ABW					
ACO					
AEI					
AEL	1.02925e-06	5.76291e-06	3.15411e-05	6.11937e-07	5.76291e-06
AEN					
AET	3.80125e-07	1.1248e-06	3.24202e-06	2.83006e-07	1.1248e-06
AFG					
AFI	6.47075e-07	2.65018e-06	1.07483e-05	4.65507e-07	2.65018e-06
AFN					
AFO	1.01976e-06	6.73942e-06	4.04835e-05	6.26473e-07	6.73942e-06
AFR	9.20765e-07	3.12673e-06	1.1752e-05	6.31029e-07	3.12673e-06
AFS	7.56737e-07	2.05153e-06	9.57473e-06	5.66368e-07	2.05153e-06
AFT					
AFX					
AFY	1.40672e-06	3.17529e-06	1.17134e-05	8.94384e-07	3.17529e-06
AHT					
ANA					
APC					
APD					
AST				3.32091e-109	
ASV	1.2724e-06	0	1.25296e-05	6.999e-07	
ATN	1.42866e-06	1.49934e-36	6.03895e-05	4.57266e-07	
ATO	9.1619e-07	7.36169e-06	3.39389e-05	5.81137e-07	7.36169e-06
ATS	7.84397e-07	3.04923e-06	1.45272e-05	5.75711e-07	3.04923e-06
ATT					
ATV					
AWO					
AWW	1.61363e-06	1.34721e-27	7.35024e-05		
BCT					
BEA	1.15599e-06	5.44094e-06	2.447e-05	8.3709e-07	5.44094e-06
BEC	1.10442e-06	5.09553e-06	2.32609e-05	8.0404e-07	5.09553e-06
BIK					
BOF	1.61937e-06	2.06658e-104	3.86649e-05	9.61326e-07	
BOG	1.11181e-06	4.92065e-06	1.9423e-05	7.82112e-07	4.92065e-06
BOZ	9.42345e-07	2.73706e-06	8.50675e-06	6.85356e-07	2.73706e-06
BPH	1.04235e-06	3.84634e-06	1.48961e-05	7.40529e-07	3.84634e-06
BRE					
BSV	1.41695e-06	6.34314e-11	7.02698e-06		
CAN	8.43648e-07	6.03427e-06	2.94663e-05	5.62701e-07	6.03427e-06
CAS					
CDO					
CFI	6.03028e-07	2.08562e-06	7.98522e-06	4.11179e-07	2.08562e-06
CGF					
CGS	1.28443e-06	2.0031e-30	3.32325e-05	7.9845e-07	
CHA					
CON	1.142e-06	4.99663e-06	2.12541e-05	8.07826e-07	4.99663e-06
CZP					
DAC					
DDR					
DFO	1.1017e-06	4.51806e-06	1.75227e-05	7.82411e-07	4.51806e-06
DFT					
DOH					
DON	4.80431e-07	1.49802e-06	4.46297e-06	3.55622e-07	1.49802e-06

EAB					
EDI					
EMT	7.18207e-07	1.94075e-06	5.77746e-06	5.60437e-07	1.94075e-06
EON	4.43393e-07	1.91256e-06	8.24792e-06	3.17328e-07	1.91256e-06
EPI					
ERI					
ESV					
ETR	4.1463e-07	9.21965e-07	2.41578e-06	2.88318e-07	9.21965e-07
EUO	1.04972e-06	5.75126e-06	3.34914e-05	6.862e-07	5.75126e-06
EZT	1.12927e-06	6.71542e-06	3.299e-05	7.64733e-07	6.71542e-06
FAR					
FAU	6.95549e-07	1.75777e-06	4.79472e-06	5.43667e-07	1.75777e-06
FER	9.22181e-07	4.73249e-06	1.88136e-05	5.23801e-07	4.73249e-06
FRA					
GIS					
GIU					
GME	6.20983e-07	2.24534e-06	8.41382e-06	4.42014e-07	2.24534e-06
GON	7.28363e-07	4.26444e-06	2.03602e-05	4.81671e-07	4.26444e-06
GOO					
HEU					
IFR	1.2065e-06	6.31719e-06	3.19912e-05	8.23274e-07	6.31719e-06
IHW					
IMF	1.33581e-06	8.27227e-06	3.85582e-05	8.68393e-07	8.27227e-06
IRR	8.56789e-07	2.35338e-06	6.49192e-06	6.70074e-07	2.35338e-06
ISV	1.07416e-06	4.6866e-06	2.05648e-05	7.85879e-07	4.6866e-06
ITE	1.40169e-06	7.20077e-151	3.37352e-05		
ITH	1.36511e-06	6.38477e-06	3.06254e-05	8.3628e-07	6.38477e-06
ITR	1.3651e-06	6.34461e-06	3.06651e-05	8.36555e-07	6.34461e-06
ITW					
IWR	1.17441e-06	5.22729e-06	2.2949e-05	8.29434e-07	5.22729e-06
IWS	9.5371e-07	3.62967e-06	1.45035e-05	7.07935e-07	3.62967e-06
IWV	7.67501e-07	2.38401e-06	7.86184e-06	5.60163e-07	2.38401e-06
IWW	1.08611e-06	5.5114e-06	2.62746e-05	7.51661e-07	5.5114e-06
JBW					
JOZ					
JRY	1.80316e-06	0	2.04097e-05	8.48763e-07	
JSN					
JST	1.49574e-06	0	1.08368e-05	9.4133e-07	
JSW					
KFI	1.26673e-06	6.41955e-10	3.45887e-05		
LAU					
LEV					
LIO					
LOS					
LOV					
LTA	9.97226e-07	0	1.1482e-05		
LTF	3.69889e-07	1.54173e-06	6.70134e-06	2.5216e-07	1.54173e-06
LTJ					
LTL	6.05262e-07	2.04492e-06	9.06047e-06	4.32013e-07	2.04492e-06
LTN					
MAR					
MAZ	3.48127e-07	1.37536e-06	5.45887e-06	2.52725e-07	1.37536e-06
MEI	1.17476e-06	3.88855e-06	1.56489e-05	8.07942e-07	3.88855e-06
MEL	1.33115e-06	8.33286e-06	3.92593e-05	8.87241e-07	8.33286e-06
MEP					
MER	1.12329e-06	2.83958e-08	1.21958e-05	7.01005e-07	
MFI	1.37451e-06	8.4874e-06	3.87992e-05	8.9005e-07	8.4874e-06
MFS	1.04381e-06	5.95247e-06	3.1384e-05	6.73174e-07	5.95247e-06

MON					
MOR	6.1378e-07	2.84615e-06	1.34063e-05	4.13172e-07	2.84615e-06
MOZ	4.28642e-07	1.81965e-06	8.15553e-06	3.03889e-07	1.81965e-06
MRE	8.761e-07	7.25228e-06	4.18648e-05	5.68669e-07	7.25228e-06
MSE	1.07435e-06	5.37188e-06	2.5748e-05	7.64294e-07	5.37188e-06
MSO					
MTF	1.07297e-06	1.87302e-76	5.99055e-05		
MTN					
MTT	1.0166e-06	7.04085e-06	4.20009e-05	6.36083e-07	7.04085e-06
MTW	7.54624e-07	4.53886e-06	2.22188e-05	5.04216e-07	4.53886e-06
MVY					
MWW	1.49399e-06	8.37288e-06	4.52682e-05	9.81548e-07	8.37288e-06
NAB					
NAT					
NES	8.91952e-07	3.99585e-06	2.09475e-05	6.6123e-07	3.99585e-06
NON					
NPO	1.11633e-06	6.1042e-43	8.00108e-06	5.59284e-07	6.1042e-43
NPT					
NSI					
OBW	6.79399e-07	1.78583e-06	4.81487e-06	5.09249e-07	1.78583e-06
OFF	6.77685e-07	3.43695e-06	1.57986e-05	4.76466e-07	3.43695e-06
OSI	6.084e-07	3.36436e-06	1.66646e-05	4.15296e-07	3.36436e-06
OSO	1.05342e-06	3.08019e-06	1.01655e-05	7.53974e-07	3.08019e-06
OWE					
PCR	9.26573e-07	9.06232e-11	1.53293e-05		
PHI					
PON	1.37909e-06	1.33557e-26	1.60448e-05	7.70823e-07	1.33557e-26
PUN	1.445e-06	4.79653e-06	1.85645e-05	9.2312e-07	4.79653e-06
RHO	1.65611e-06	1.40951e-63	9.66031e-06		
RRO	1.29158e-06	1.5899e-07	6.32131e-06		
RSN					
RTE	1.6071e-06	1.11864e-35	7.73687e-05		
RTH	1.38135e-06	1.89888e-144	3.26701e-05		
RUT					
RWR					
RWY	1.08595e-06	1.96164e-06	3.70041e-06	9.06809e-07	1.96164e-06
SAF	5.27991e-07	2.46464e-06	1.06077e-05	3.70775e-07	2.46464e-06
SAO	9.82881e-07	3.30974e-06	1.15883e-05	7.42769e-07	3.30974e-06
SAS	1.32795e-06	5.95773e-69	3.11298e-05		
SAT					
SAV	8.096e-07	1.78229e-20	1.39439e-05		
SBE	1.04682e-06	1.62166e-06	7.66196e-06	4.82197e-07	1.62166e-06
SBN					
SBS	8.57416e-07	2.28974e-06	6.61662e-06	6.16939e-07	2.28974e-06
SBT	8.56546e-07	2.30437e-06	6.68655e-06	6.1953e-07	2.30437e-06
SFE	7.09981e-07	3.10183e-06	1.44988e-05	4.92697e-07	3.10183e-06
SFF	1.12502e-06	5.37988e-06	2.69003e-05	7.57162e-07	5.37988e-06
SFG	8.95696e-07	4.91127e-06	2.4309e-05	6.06435e-07	4.91127e-06
SFH	5.96419e-07	2.12909e-06	7.91355e-06	4.33733e-07	2.12909e-06
SFN	5.86416e-07	2.10351e-06	7.75975e-06	4.23782e-07	2.10351e-06
SFO	9.20459e-07	3.19581e-06	1.21178e-05	6.36783e-07	3.19581e-06
SFS	1.15219e-06	5.90162e-06	2.43051e-05	7.85264e-07	5.90162e-06
SFV	1.2945e-06	7.96173e-06	3.65752e-05	8.60683e-07	7.96173e-06
SGT					
SIV					
SOD					
SOF	1.13442e-06	9.41759e-08	9.84706e-06	5.83396e-07	

SOS	4.57615e-07	5.58675e-11	5.81715e-07		
SSF	7.1754e-07	3.11553e-06	1.22852e-05	5.19901e-07	3.11553e-06
SSY	7.23583e-07	3.16423e-06	1.4876e-05	5.0161e-07	3.16423e-06
STF	1.21401e-06	5.63727e-06	2.89742e-05	8.23461e-07	5.63727e-06
STI	1.47683e-06	8.55132e-06	5.10269e-05	9.6582e-07	8.55132e-06
STO	6.29419e-07	3.10926e-06	1.3511e-05	4.34585e-07	3.10926e-06
STW	1.77675e-06	7.50783e-06	4.56611e-05	1.12777e-06	7.50783e-06
SZR	9.33502e-07	5.23177e-06	2.56357e-05	6.03545e-07	5.23177e-06
TER	1.44246e-06	7.24419e-06	3.38597e-05	9.18497e-07	7.24419e-06
THO					
TOL					
TON	1.12423e-06	7.88577e-06	4.21601e-05	6.92381e-07	7.88577e-06
TSC	6.81321e-07	2.24305e-10	4.88182e-06	5.59955e-07	2.24305e-10
TUN	1.25289e-06	7.51066e-06	3.77287e-05	8.32919e-07	7.51066e-06
UEI					
UFI					
UOS	1.31822e-06	1.77799e-32	1.9352e-05		
UOZ					
USI	1.12101e-06	4.06762e-06	1.84433e-05	7.64069e-07	4.06762e-06
UTL	8.41144e-07	3.17423e-06	1.041e-05	6.12305e-07	3.17423e-06
UWY	1.37343e-06	5.6631e-06	2.78485e-05	8.81563e-07	5.6631e-06
VET	5.35192e-07	2.92653e-06	1.46703e-05	3.64804e-07	2.92653e-06
VFI	4.47501e-07	9.61578e-07	2.06825e-06	3.50612e-07	9.61578e-07
VNI					
VSV					
WEI					
YUG					
ZON					

Table S7. Henry coefficients of the targeted gas molecules in the set of Zeolitic Imidazolate Frameworks.

	ZIFs				
	Ar	**O_2**	**CO_2**	**N_2**	**CH_4**
ABW	2.06493e-06	2.16352e-06	1.9722e-05	1.86721e-06	5.03833e-06
ACO	1.63236e-06	1.57717e-06	1.03347e-05	1.27488e-06	3.31014e-06
AEI	1.70291e-06	1.76179e-06	1.58465e-05	1.5527e-06	3.68799e-06
AEL	2.78099e-06	3.0097e-06	9.8236e-05	2.36452e-06	8.71278e-06
AEN	1.70291e-06	1.84359e-06	6.79655e-05	1.37624e-06	3.95086e-06
AET	1.97618e-06	2.25e-06	0.00035269	1.61026e-06	4.44623e-06
AFG	2.04603e-06	2.17049e-06	3.8171e-05	1.87418e-06	4.86473e-06
AFI	3.01246e-06	3.28304e-06	0.00010341	2.786e-06	8.91612e-06
AFN	2.12154e-06	2.28575e-06	0.00011281	1.91946e-06	5.15905e-06
AFO	2.51965e-06	2.78748e-06	7.70693e-05	2.22496e-06	7.96149e-06
AFR	2.27103e-06	2.41181e-06	6.19675e-05	2.04669e-06	6.48199e-06
AFS	1.85964e-06	1.94399e-06	1.99185e-05	1.6466e-06	3.91084e-06
AFT	1.71149e-06	1.77926e-06	2.2143e-05	1.57153e-06	3.79756e-06
AFX	1.75842e-06	1.83274e-06	2.23201e-05	1.62805e-06	3.9652e-06
AFY	1.50849e-06	1.52453e-06	1.35244e-05	1.34348e-06	2.78541e-06
AHT	1.99941e-06	2.20199e-06	0.00063117	1.73501e-06	5.49636e-06
ANA	1.63884e-06	1.69908e-06	9.19815e-06	1.44604e-06	3.75568e-06
APC	2.19017e-06	2.335e-06	4.51588e-05	2.05417e-06	5.61159e-06
APD	2.22107e-06	2.42001e-06	8.22753e-05	2.01107e-06	6.73415e-06
AST	2.29627e-06	2.37148e-06	1.72718e-05	1.87776e-06	8.42917e-06
ASV	1.94172e-06	2.17568e-06	0.0001277	1.48595e-06	4.44122e-06
ATN	2.01114e-06	2.10861e-06	2.12216e-05	1.75312e-06	4.56853e-06
ATO	1.92655e-06	2.08948e-06	7.6287e-05	1.7146e-06	5.59718e-06
ATS	1.94452e-06	2.09709e-06	3.94806e-05	1.73783e-06	4.76407e-06
ATT	1.85097e-06	1.93125e-06	1.69275e-05	1.62748e-06	4.16197e-06
ATV	2.17309e-06	2.40704e-06	0.00017467	1.8956e-06	6.57679e-06
AWO	1.89159e-06	1.99062e-06	3.03726e-05	1.68502e-06	4.64392e-06
AWW	2.00557e-06	2.12504e-06	2.98397e-05	1.83445e-06	4.90962e-06
BCT	1.74101e-06	1.82044e-06	1.2375e-05	1.34653e-06	3.83408e-06
BEA	2.68908e-06	2.88632e-06	0.00019764	2.32286e-06	8.18059e-06
BEC	2.49373e-06	2.65164e-06	4.96379e-05	2.12282e-06	6.50505e-06
BIK	2.34632e-06	2.47083e-06	3.92952e-05	1.88264e-06	6.12603e-06
BOF	1.90145e-06	2.03415e-06	2.51089e-05	1.55507e-06	5.08703e-06
BOG	2.28444e-06	2.41351e-06	4.21933e-05	1.85223e-06	5.45422e-06
BOZ	1.67087e-06	1.72482e-06	1.39927e-05	1.53463e-06	2.85006e-06
BPH	2.15907e-06	2.29504e-06	4.38711e-05	1.86875e-06	5.14702e-06
BRE	1.97711e-06	2.02057e-06	1.94969e-05	1.51235e-06	4.73312e-06
BSV	1.39801e-06	1.49944e-06	1.67557e-05	1.21608e-06	2.62287e-06
CAN	1.86865e-06	2.00341e-06	3.07472e-05	1.70839e-06	4.27794e-06
CAS	2.25076e-06	2.40722e-06	5.7024e-05	1.76982e-06	5.70761e-06
CDO	1.97874e-06	2.12898e-06	7.30602e-05	1.56277e-06	5.24763e-06
CFI	2.03646e-06	2.17233e-06	5.04536e-05	1.66942e-06	5.00029e-06
CGF	1.32172e-06	1.39878e-06	3.87701e-05	1.03325e-06	2.48643e-06
CGS	1.76997e-06	1.83892e-06	1.46675e-05	1.55995e-06	4.14036e-06
CHA	1.82953e-06	1.90934e-06	2.72136e-05	1.70698e-06	4.3825e-06
CON	1.94138e-06	2.08342e-06	6.11248e-05	1.59893e-06	4.07396e-06
CZP	1.16791e-06	1.1918e-06	1.43808e-05	9.34987e-07	2.35789e-06
DAC	2.11023e-06	2.24591e-06	4.56619e-05	1.68659e-06	4.80595e-06
DDR	1.79697e-06	1.89456e-06	2.81773e-05	1.4743e-06	3.72491e-06
DFO	1.80296e-06	1.96594e-06	7.13774e-05	1.59169e-06	3.91086e-06
DFT	2.23449e-06	2.36399e-06	0.00020722	2.11925e-06	6.28201e-06
DOH	1.94232e-06	2.07089e-06	3.18628e-05	1.69133e-06	4.69848e-06

DON	2.97388e-06	3.25813e-06	9.34849e-05	2.80735e-06	9.48228e-06
EAB	1.69987e-06	1.7725e-06	2.27061e-05	1.54894e-06	3.92411e-06
EDI	1.57799e-06	1.67327e-06	8.71795e-05	1.48024e-06	3.09996e-06
EMT	1.81932e-06	1.88815e-06	1.41819e-05	1.66849e-06	3.73111e-06
EON	2.04312e-06	2.14504e-06	4.68951e-05	1.69376e-06	4.74779e-06
EPI	1.59832e-06	1.70741e-06	5.25879e-05	1.31109e-06	3.09236e-06
ERI	1.94819e-06	2.05917e-06	3.97834e-05	1.74455e-06	4.40501e-06
ESV	1.81165e-06	1.92001e-06	1.98502e-05	1.62423e-06	3.99537e-06
ETR	1.84829e-06	1.90987e-06	2.04152e-05	1.58146e-06	3.9739e-06
EUO	2.10013e-06	2.25688e-06	4.99624e-05	1.74363e-06	5.49363e-06
EZT	2.1068e-06	2.26566e-06	4.50044e-05	1.78195e-06	5.35075e-06
FAR	1.66163e-06	1.73907e-06	1.51494e-05	1.52008e-06	3.65199e-06
FAU	1.82877e-06	1.89771e-06	1.40655e-05	1.67889e-06	3.7825e-06
FER	2.1718e-06	2.27922e-06	5.98431e-05	1.66872e-06	5.84893e-06
FRA	1.63221e-06	1.70933e-06	1.36151e-05	1.49983e-06	3.54664e-06
GIS	1.71544e-06	1.77833e-06	2.15959e-05	1.5931e-06	3.81553e-06
GIU	1.79716e-06	1.90203e-06	2.13097e-05	1.66232e-06	4.26448e-06
GME	1.98804e-06	2.09698e-06	2.9472e-05	1.75571e-06	4.31701e-06
GON	2.26112e-06	2.46723e-06	6.05323e-05	1.9016e-06	6.03414e-06
GOO	1.88062e-06	2.0279e-06	6.15998e-05	1.67809e-06	4.18368e-06
HEU	2.20574e-06	2.40734e-06	9.53516e-05	1.79351e-06	4.98155e-06
IFR	2.04791e-06	2.24105e-06	0.00012284	1.73255e-06	5.43679e-06
IHW	2.02223e-06	2.19644e-06	8.50433e-05	1.52409e-06	5.00411e-06
IMF	1.86009e-06	2.01934e-06	6.08973e-05	1.47991e-06	4.36588e-06
IRR	2.40488e-06	2.57902e-06	3.90007e-05	2.08326e-06	5.56142e-06
ISV	2.11278e-06	2.22934e-06	4.64891e-05	1.81808e-06	5.15444e-06
ITE	2.04335e-06	2.15704e-06	3.98337e-05	1.76605e-06	5.17214e-06
ITH	2.05411e-06	2.23227e-06	5.09277e-05	1.73093e-06	4.79269e-06
ITR	2.06832e-06	2.24856e-06	5.09094e-05	1.74033e-06	4.80153e-06
ITW	2.08777e-06	2.11545e-06	2.36028e-05	1.68904e-06	5.2157e-06
IWR	2.15944e-06	2.39493e-06	7.35498e-05	1.89373e-06	5.19086e-06
IWS	2.21583e-06	2.34267e-06	4.73575e-05	1.86576e-06	5.27784e-06
IWV	1.90342e-06	2.05766e-06	4.93921e-05	1.53171e-06	4.53846e-06
IWW	2.08382e-06	2.24156e-06	4.70105e-05	1.77826e-06	5.17759e-06
JBW	2.01406e-06	2.11806e-06	6.59429e-05	1.71095e-06	4.55618e-06
JOZ	1.72278e-06	1.80309e-06	2.43898e-05	1.54283e-06	3.30778e-06
JRY	2.04334e-06	2.21018e-06	7.02367e-05	1.70912e-06	4.88492e-06
JSN	2.07221e-06	2.19758e-06	6.11251e-05	1.79392e-06	5.80671e-06
JST	1.65684e-06	1.69995e-06	9.56162e-06	1.49904e-06	2.92288e-06
JSW	2.1926e-06	2.3841e-06	9.4773e-05	2.02502e-06	5.94672e-06
KFI	1.67128e-06	1.71556e-06	1.04456e-05	1.5007e-06	3.47861e-06
LAU	2.22393e-06	2.40234e-06	4.18423e-05	1.86255e-06	5.99934e-06
LEV	1.90028e-06	1.99207e-06	2.21978e-05	1.72558e-06	4.3131e-06
LIO	1.74104e-06	1.82988e-06	1.85212e-05	1.60057e-06	4.04244e-06
LOS	2.10218e-06	2.21079e-06	2.67113e-05	1.89819e-06	4.84499e-06
LOV	1.74425e-06	1.82467e-06	3.73476e-05	1.56033e-06	3.79723e-06
LTA	1.92783e-06	1.93402e-06	2.00146e-05	1.53533e-06	4.09539e-06
LTF	2.03902e-06	2.1734e-06	7.05088e-05	1.76559e-06	4.52954e-06
LTJ	1.69306e-06	1.81516e-06	4.53003e-05	1.41679e-06	3.25077e-06
LTL	2.15133e-06	2.28733e-06	9.34786e-05	1.92508e-06	5.20108e-06
LTN	1.80071e-06	1.88696e-06	2.04826e-05	1.64698e-06	4.34173e-06
MAR	1.86229e-06	1.97362e-06	3.53367e-05	1.6948e-06	4.35793e-06
MAZ	1.88224e-06	1.97918e-06	3.49877e-05	1.51055e-06	3.90409e-06
MEI	1.83624e-06	1.89835e-06	4.60675e-05	1.61589e-06	5.15571e-06
MEL	2.64842e-06	2.83717e-06	6.56087e-05	2.20324e-06	7.41804e-06
MEP	1.70293e-06	1.82638e-06	7.08751e-05	1.3796e-06	3.56624e-06
MER	1.60952e-06	1.68599e-06	1.28414e-05	1.47002e-06	3.33451e-06
MFI	2.1523e-06	2.3635e-06	6.75733e-05	1.73461e-06	5.94007e-06

MFS	2.54633e-06	2.73891e-06	7.5905e-05	2.13329e-06	6.97987e-06
MON	1.71287e-06	1.79491e-06	3.44895e-05	1.31409e-06	3.09118e-06
MOR	1.87694e-06	2.0024e-06	7.04388e-05	1.5226e-06	3.94057e-06
MOZ	1.99523e-06	2.12296e-06	7.79957e-05	1.72697e-06	4.57953e-06
MRE	2.27578e-06	2.44575e-06	5.42139e-05	1.88754e-06	6.65595e-06
MSE	2.73421e-06	2.9437e-06	8.35734e-05	2.41692e-06	7.88258e-06
MSO	2.46271e-06	2.70523e-06	6.78994e-05	2.21438e-06	7.2674e-06
MTF	1.802e-06	1.89956e-06	0.00013967	1.41942e-06	4.632e-06
MTN	1.93164e-06	2.06671e-06	2.94792e-05	1.64192e-06	4.59899e-06
MTT	2.08392e-06	2.26424e-06	0.00017146	1.6337e-06	5.28797e-06
MTW	2.11561e-06	2.26067e-06	7.8521e-05	1.6585e-06	5.10298e-06
MVY	3.18657e-06	3.72306e-06	0.00026237	2.76783e-06	1.05527e-05
MWW	2.41782e-06	2.64365e-06	0.00010335	2.06057e-06	6.44424e-06
NAB	1.56103e-06	1.61993e-06	1.13219e-05	1.41439e-06	2.86446e-06
NAT	1.61051e-06	1.67483e-06	1.17126e-05	1.44724e-06	3.28526e-06
NES	1.75654e-06	1.90005e-06	8.36032e-05	1.4472e-06	4.14084e-06
NON	2.07433e-06	2.22827e-06	4.20256e-05	1.73544e-06	5.68905e-06
NPO	2.52016e-06	2.78958e-06	0.00020587	2.54407e-06	7.65871e-06
NPT	1.75454e-06	1.82553e-06	1.76645e-05	1.61978e-06	3.08141e-06
NSI	1.75467e-06	1.80575e-06	2.28374e-05	1.29301e-06	3.86761e-06
OBW	1.65834e-06	1.70641e-06	1.44803e-05	1.53662e-06	2.76059e-06
OFF	2.06491e-06	2.18797e-06	4.00604e-05	1.80521e-06	4.76002e-06
OSI	2.41929e-06	2.54772e-06	3.36503e-05	2.11177e-06	6.36119e-06
OSO	1.84376e-06	1.92714e-06	1.30132e-05	1.71389e-06	3.19266e-06
OWE	2.28549e-06	2.51359e-06	0.00017566	2.1599e-06	6.23768e-06
PCR	2.09073e-06	2.25881e-06	4.70975e-05	1.64111e-06	4.94008e-06
PHI	1.61263e-06	1.66137e-06	1.14163e-05	1.45667e-06	3.31235e-06
PON	1.94138e-06	2.11528e-06	8.80226e-05	1.73556e-06	4.71539e-06
PUN	1.65805e-06	1.70747e-06	1.095e-05	1.49124e-06	3.16803e-06
RHO	1.72817e-06	1.78254e-06	9.29747e-06	1.55334e-06	3.31695e-06
RRO	2.42708e-06	2.55178e-06	5.27665e-05	1.89582e-06	6.3163e-06
RSN	1.71391e-06	1.78649e-06	3.3581e-05	1.4949e-06	3.70146e-06
RTE	2.03592e-06	2.15286e-06	5.52763e-05	1.64816e-06	4.24762e-06
RTH	2.05573e-06	2.17383e-06	4.74987e-05	1.7633e-06	5.06334e-06
RUT	1.72993e-06	1.83079e-06	2.14529e-05	1.4364e-06	3.66468e-06
RWR	2.29739e-06	2.50152e-06	6.63968e-05	2.00844e-06	6.58526e-06
RWY	2.40135e-06	2.50448e-06	3.37126e-05	2.33303e-06	3.43399e-06
SAF	2.62126e-06	2.87555e-06	8.98325e-05	2.23612e-06	7.95994e-06
SAO	1.84817e-06	1.96605e-06	2.15558e-05	1.70425e-06	4.07866e-06
SAS	1.89962e-06	2.00553e-06	3.42714e-05	1.72167e-06	4.44368e-06
SAT	1.97946e-06	2.08183e-06	2.82271e-05	1.80463e-06	5.00811e-06
SAV	1.64418e-06	1.68955e-06	9.87363e-06	1.47234e-06	3.39692e-06
SBE	1.9005e-06	2.01097e-06	2.60964e-05	1.69841e-06	3.92305e-06
SBN	1.48377e-06	1.5261e-06	9.99362e-06	1.33462e-06	2.85729e-06
SBS	2.07871e-06	2.20527e-06	2.8793e-05	1.82229e-06	4.50664e-06
SBT	2.0417e-06	2.15836e-06	2.79522e-05	1.78389e-06	4.35905e-06
SFE	1.87728e-06	2.0548e-06	8.95474e-05	1.43568e-06	3.98449e-06
SFF	1.975e-06	2.14392e-06	8.16427e-05	1.68815e-06	5.41809e-06
SFG	2.59283e-06	2.81472e-06	6.67633e-05	2.25355e-06	7.52956e-06
SFH	1.94748e-06	2.1022e-06	7.54589e-05	1.63295e-06	4.84702e-06
SFN	2.05247e-06	2.20394e-06	7.95611e-05	1.7882e-06	5.30862e-06
SFO	2.25082e-06	2.39957e-06	8.40726e-05	2.07385e-06	6.40098e-06
SFS	2.44406e-06	2.67076e-06	7.81236e-05	2.01717e-06	6.37124e-06
SFV	2.04206e-06	2.29135e-06	0.0001446	1.8058e-06	4.99746e-06
SGT	1.61447e-06	1.65637e-06	1.04133e-05	1.44475e-06	3.31626e-06
SIV	1.71644e-06	1.77749e-06	1.30006e-05	1.49194e-06	3.60799e-06
SOD	1.92402e-06	2.08054e-06	3.83207e-05	1.66909e-06	4.23975e-06

SOF	1.81233e-06	1.98223e-06	0.00017108	1.64765e-06	3.74653e-06
SOS	2.22279e-06	2.37751e-06	8.05506e-05	1.92404e-06	6.31149e-06
SSF	1.53668e-06	1.73725e-06	0.00273274	1.67376e-06	3.58221e-06
SSY	2.13539e-06	2.25106e-06	5.06393e-05	1.74684e-06	5.35901e-06
STF	2.08053e-06	2.24731e-06	0.00017118	1.93119e-06	5.56688e-06
STI	2.64e-06	2.88173e-06	7.2173e-05	2.32421e-06	8.22982e-06
STO	2.0572e-06	2.19545e-06	4.21993e-05	1.76296e-06	5.15591e-06
STW	1.70478e-06	1.78867e-06	5.49025e-05	1.43822e-06	3.35713e-06
SZR	2.0812e-06	2.1816e-06	3.68947e-05	1.71445e-06	5.13563e-06
TER	2.41248e-06	2.6574e-06	9.00933e-05	2.11099e-06	6.92544e-06
THO	1.64971e-06	1.75789e-06	2.59884e-05	1.50459e-06	3.23474e-06
TOL	1.73981e-06	1.82623e-06	1.84807e-05	1.60071e-06	4.03975e-06
TON	2.35421e-06	2.54277e-06	8.43833e-05	1.94246e-06	6.80939e-06
TSC	1.86352e-06	1.95855e-06	4.53772e-05	1.74279e-06	4.4247e-06
TUN	1.92457e-06	2.08257e-06	6.78234e-05	1.4859e-06	4.37754e-06
UEI	1.7317e-06	1.79042e-06	1.96257e-05	1.50646e-06	4.11312e-06
UFI	1.85489e-06	1.92253e-06	3.08036e-05	1.62895e-06	4.44498e-06
UOS	2.01265e-06	2.08482e-06	2.93657e-05	1.69137e-06	4.87631e-06
UOZ	1.82317e-06	1.95861e-06	0.00013123	1.35423e-06	3.63697e-06
USI	2.03446e-06	2.24131e-06	0.00029539	1.70729e-06	5.39013e-06
UTL	2.12778e-06	2.31129e-06	8.9773e-05	1.74197e-06	5.26847e-06
UWY	2.23813e-06	2.44193e-06	6.79057e-05	1.91395e-06	5.64319e-06
VET	1.74762e-06	1.94176e-06	0.00010685	1.36842e-06	4.15298e-06
VFI	2.15684e-06	2.3935e-06	0.00041256	1.99809e-06	5.52215e-06
VNI	1.72381e-06	1.79951e-06	2.44645e-05	1.46271e-06	3.41122e-06
VSV	1.55379e-06	1.61376e-06	1.52276e-05	1.31548e-06	3.06565e-06
WEI	1.6633e-06	1.7781e-06	0.00011706	1.58554e-06	3.48537e-06
YUG	2.1647e-06	2.3118e-06	4.4457e-05	1.87536e-06	4.93251e-06
ZON	2.24268e-06	2.43824e-06	9.506e-05	2.05758e-06	6.9086e-06

[1] T. F. Willems, C. H. Rycro, M. Kazi, J. C. Meza and M. Haranczyk, *Microporous Mesoporous Mater.*, 2012, **149**, 134.