

Electronic Supplementary Information

Reducing possible combinations of Wyckoff positions for zeolite structure prediction

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Table S1 TAD densities for 221 known zeolite structures.

Zeolite	Space group	TAD density									
		222	$\bar{4}$	$\bar{4}_2m$	$\bar{4}_3m$	2 (T nm ⁻¹)	3 (T nm ⁻¹)	2mm (T nm ⁻¹)	3m (T nm ⁻¹)	m (T nm ⁻²)	1 (T nm ⁻³)
ABW	<i>Imma</i>	—	—	—	—	0	—	0	—	4.805	0
ACO	<i>Im$\bar{3}m$</i>	—	—	0	—	0	—	0	2.356	0	0
AEI	<i>Cmcm</i>	—	—	—	—	0	—	0	—	0	15.57
AEL	<i>Imma</i>	—	—	—	—	0	—	0	—	3.586	15.47
AEN	<i>Cmce</i>	—	—	—	—	0	—	—	—	0	20.38
AET	<i>Cmcm</i>	—	—	—	—	0	—	0	—	3.268	15.90
AFG	<i>P6₃/mmc</i>	—	—	—	—	1.614	—	0	0	4.513	8.734
AFI	<i>P6/mcc</i>	0	—	—	—	0	0	—	—	0	17.49
AFN	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	17.96
AFO	<i>Cmcm</i>	—	—	—	—	0	—	0	—	5.636	7.794
AFR	<i>Pmmn</i>	—	—	—	—	—	—	0	—	0	15.48
AFS	<i>P6₃/mcm</i>	—	—	—	—	0	1.540	0	0	0	12.73
AFT	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	0	15.60
AFV	<i>P$\bar{3}m$1</i>	—	—	—	—	1.522	—	—	0	0	12.90
AFX	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	0	15.61
AFY	<i>P$\bar{3}1m$</i>	—	—	—	—	0	2.325	—	0	0	10.59
AHT	<i>Cmcm</i>	—	—	—	—	0	—	0	—	4.946	12.57
ANA	<i>Ia$\bar{3}d$</i>	0	0	—	—	1.054	0	—	—	—	0
APC	<i>Cmce</i>	—	—	—	—	0	—	—	—	0	18.15
APD	<i>Cmce</i>	—	—	—	—	0	—	—	—	0	18.67
AST	<i>Fm$\bar{3}m$</i>	—	—	—	1	—	—	0	0.8579	0	0
ASV	<i>P4/mcc</i>	1	—	—	—	0	—	—	—	0	16.08
ATN	<i>I4/mmm</i>	—	—	0	—	0	—	0	—	4.757	0
ATO	<i>R$\bar{3}m$</i>	—	—	—	—	0	—	—	0	0	19.37
ATS	<i>Cmcm</i>	—	—	—	—	0	—	0	—	4.306	0
ATT	<i>Pmma</i>	—	—	—	—	0	—	0	—	4.428	11.79
ATV	<i>Cmme</i>	0	—	—	—	0	—	0	—	4.979	13.18
AVL	<i>P$\bar{3}m$1</i>	—	—	—	—	1.511	—	—	0	0	13.70
AWO	<i>Cmce</i>	—	—	—	—	0	—	—	—	0	18.55
AWW	<i>P4/nmm</i>	—	—	0	—	1.046	—	0	—	0	11.50
BCT	<i>I4/mmm</i>	—	—	0	—	0	—	1.603	—	0	0
BEA	<i>P4₁22</i>	—	—	—	—	1.135	—	—	—	—	13.74
BEC	<i>P4₂/mmc</i>	—	—	0	—	1.121	—	0	—	2.435	7.718
BIK	<i>Cmcm</i>	—	—	—	—	0	—	0.6250	—	3.360	0
BOF	<i>Pnma</i>	—	—	—	—	—	—	—	—	0	18.54
BOG	<i>Imma</i>	—	—	—	—	0	—	0	—	0	16.12
BOZ	<i>Cmcm</i>	—	—	—	—	1.405	—	0.2761	—	0.7836	8.809
BPH	<i>P$\bar{6}2m$</i>	—	—	—	—	—	1.541	0	0	0	12.72
BRE	<i>P2₁/m</i>	—	—	—	—	—	—	—	—	0	18.43
BSV	<i>Ia$\bar{3}d$</i>	0	0	—	—	0	0	—	—	—	18.25
CAN	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	4.529	0
CAS	<i>Cmcm</i>	—	—	—	—	0	—	0	—	5.067	0
CDO	<i>Cmcm</i>	—	—	—	—	0	—	0.5351	—	2.876	8.307
CFI	<i>Imma</i>	—	—	—	—	0	—	0.7767	—	3.365	0
CGF	<i>C2/m</i>	—	—	—	—	1.166	—	—	—	0	16.68
CGS	<i>Pnma</i>	—	—	—	—	—	—	—	—	0	17.11
CHA	<i>R$\bar{3}m$</i>	—	—	—	—	0	—	—	0	0	15.59
CON	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	16.06
CSV	<i>P$\bar{1}$</i>	—	—	—	—	—	—	—	—	—	16.23
CZP	<i>P6₁22</i>	—	—	—	—	1.228	—	—	—	—	10.29
DAC	<i>C2/m</i>	—	—	—	—	0	—	—	—	2.260	12.11

Zeolite	Space group	TAD density									
		222	$\bar{4}$	$\bar{4}2m$	$\bar{4}3m$	2 (T nm ⁻¹)	3 (T nm ⁻¹)	2mm (T nm ⁻¹)	3m (T nm ⁻¹)	m (T nm ⁻²)	1 (T nm ⁻³)
DDR	$R\bar{3}m$	—	—	—	—	1.453	—	—	0.9852	1.240	5.404
DFO	$P6/mmm$	—	—	—	—	—	—	0	0	2.884	13.72
DFT	$P4_2/mmc$	—	—	0	—	0	—	0	—	6.522	0
DOH	$P6/mmm$	—	—	—	—	—	—	0.8242	1.784	2.547	0
DON	$Cmcm$	—	—	—	—	0	—	0	—	4.001	12.73
EAB	$P6_3/mmc$	—	—	—	—	1.540	—	0	0	0	10.99
EDI	$P4_2m2$	—	—	1	—	0	—	0	—	2.288	0
EEI	$Fmmm$	0	—	—	—	0	—	0.9014	—	3.328	8.998
EMT	$P6_3/mmc$	—	—	—	—	0	—	0	0	0	13.50
EON	$Pmmn$	—	—	—	—	—	—	0	—	2.174	11.62
EPI	$C2/m$	—	—	—	—	0	—	—	—	0	18.26
ERI	$P6_3/mmc$	—	—	—	—	0	—	0	0	4.155	11.00
ESV	$Pnma$	—	—	—	—	—	—	—	—	0	17.58
ETL	$Cmcm$	—	—	—	—	0	—	0	—	2.328	12.5
ETR	$P6_3mc$	—	—	—	—	—	—	—	0	0	15.66
EUO	$Cmme$	0	—	—	—	0	—	0	—	3.533	10.29
EWS	$Cmce$	—	—	—	—	1.265	—	—	—	0	14.48
EZT	$Imma$	—	—	—	—	1.959	—	0	—	4.444	5.803
FAR	$P6_3/mmc$	—	—	—	—	0	—	0	0	4.479	14.98
FAU	$Fd\bar{3}m$	—	—	—	0	0	—	—	0	0	13.50
FER	$Immm$	—	—	—	—	—	—	1.063	—	2.857	8.133
FRA	$P\bar{3}m1$	—	—	—	—	1.608	—	—	0	0	14.05
GIS	$I4_1/amd$	—	—	0	—	1.473	—	0	—	0	0
GIU	$P6_3/mmc$	—	—	—	—	1.611	—	0	0	4.497	13.12
GME	$P6_3/mmc$	—	—	—	—	0	—	0	0	0	15.62
GON	$C222$	0	—	—	—	0	—	—	—	—	19.35
GOO	$C222_1$	—	—	—	—	1.160	—	—	—	—	14.11
HEU	$C2/m$	—	—	—	—	1.140	—	—	—	0	15.85
IFO	$Pnnm$	—	—	—	—	0	—	—	—	0	17.34
IFR	$C2/m$	—	—	—	—	0	—	—	—	0	17.17
IFW	$C2/m$	—	—	—	—	0	—	—	—	3.678	12.24
IFY	$P4/mbm$	—	—	—	—	—	—	0	—	6.879	11.65
IHW	$Cmce$	—	—	—	—	0	—	—	—	3.695	13.55
IMF	$Cmcm$	—	—	—	—	0	—	0	—	4.254	11.98
IRN	$Immm$	—	—	—	—	—	—	1.220	—	5.010	8.237
IRR	$P6/mmm$	—	—	—	—	—	—	0	1.414	1.718	5.421
ISV	$P4_2/mmc$	—	—	0	—	0	—	0	—	2.434	11.53
ITE	$Cmcm$	—	—	—	—	0	—	0	—	0	16.41
ITG	$P2/m$	—	—	—	—	0	—	—	—	2.977	14.27
ITH	$Amm2$	—	—	—	—	—	—	0	—	3.167	12.63
ITR	$Cmcm$	—	—	—	—	0	—	0	—	3.168	12.63
ITT	$P6/mmm$	—	—	—	—	—	—	0.6103	1.744	1.064	6.750
ITW	$C2/m$	—	—	—	—	0	—	—	—	0	18.21
IWR	$Cmmm$	—	—	—	—	0	—	0	—	2.836	13.62
IWS	$I4/mmm$	—	—	0	—	1.067	—	0.5334	—	3.302	7.045
IWV	$Fmmm$	0	—	—	—	0	—	0.7192	—	2.248	9.743
IWW	$Pbam$	—	—	—	—	0	—	—	—	2.994	14.34
JBW	$Pmma$	—	—	—	—	0	—	1.247	—	3.374	0
JNT	$P2_1/c$	—	—	—	—	—	—	—	—	—	19.94
JOZ	$Pbcm$	—	—	—	—	1.408	—	—	—	0	13.12
JRY	$I2_12_12_1$	—	—	—	—	0	—	—	—	—	19.11
JSN	$P2/c$	—	—	—	—	0	—	—	—	—	17.94
JSR	$Pa\bar{3}$	—	—	—	—	—	0	—	—	—	11.99
JST	$Pa\bar{3}$	—	—	—	—	—	0	—	—	—	13.64

Zeolite	Space group	TAD density									
		222	$\bar{4}$	$\bar{4}2m$	$\bar{4}3m$	2 (T nm ⁻¹)	3 (T nm ⁻¹)	2mm (T nm ⁻¹)	3m (T nm ⁻¹)	m (T nm ⁻²)	1 (T nm ⁻³)
JSW	<i>Pbca</i>	—	—	—	—	—	—	—	—	—	18.66
KFI	<i>Im\bar{3}m</i>	—	—	0	—	0	—	0	0	0	15.47
LAU	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	18.28
LEV	<i>R\bar{3}m</i>	—	—	—	—	1.541	—	—	0	0	10.99
LIO	<i>P\bar{6}m2</i>	—	—	—	—	—	—	0	0	4.512	11.65
LOS	<i>P6₃/mmc</i>	—	—	—	—	1.613	—	0	0	4.508	0
LOV	<i>P4₂/mmc</i>	—	—	1	—	0	—	0	—	2.711	0
LTA	<i>Pm\bar{3}m</i>	—	—	—	—	—	—	0	0	2.859	0
LTF	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	2.172	11.57
LTJ	<i>P4₁2₁2</i>	—	—	—	—	0	—	—	—	0	19.00
LTL	<i>P6/mmm</i>	—	—	—	—	—	—	0	0	4.271	11.37
LTN	<i>Fd\bar{3}m</i>	—	—	—	0	0	—	—	0	0	17.12
MAR	<i>P6₃/mmc</i>	—	—	—	—	1.610	—	0	0	4.489	11.64
MAZ	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	2.149	11.45
MEI	<i>P6₃/m</i>	—	—	—	—	—	1.283	—	—	2.039	10.46
MEL	<i>\bar{I}4m2</i>	—	—	0	—	1.415	—	0	—	0	14.87
MEP	<i>Pm\bar{3}n</i>	1	—	1	—	0	1.712	0	—	1.099	0
MER	<i>I4/mmm</i>	—	—	0	—	0	—	0	—	0	16.96
MFI	<i>Pnma</i>	—	—	—	—	—	—	—	—	0	18.20
MFS	<i>Imm2</i>	—	—	—	—	—	—	0.5328	—	2.856	8.062
MON	<i>I4₁/amd</i>	—	—	0	—	0	—	0	—	3.234	0
MOR	<i>Cmcm</i>	—	—	—	—	0	—	0	—	2.201	11.80
MOZ	<i>P6/mmm</i>	—	—	—	—	—	—	0	0	4.337	11.53
MRE	<i>Imma</i>	—	—	—	—	0	—	0	—	4.756	13.22
MSE	<i>P4₂/mnm</i>	—	0	—	—	0	—	0	—	1.537	14.26
MSO	<i>R\bar{3}m</i>	—	—	—	—	1.165	—	—	0	0	14.91
MTF	<i>C2/m</i>	—	—	—	—	0.6558	—	—	—	0	19.30
MTN	<i>Fd\bar{3}m</i>	—	—	—	1	0	—	—	0.5883	1.469	0
MTT	<i>Pmmn</i>	—	—	—	—	—	—	0.8903	—	4.084	0
MTW	<i>C2/m</i>	—	—	—	—	0	—	—	—	4.781	0
MVY	<i>Pnnm</i>	—	—	—	—	0	—	—	—	4.782	13.83
MWF	<i>Im\bar{3}m</i>	—	—	0	—	1.279	—	0	0	0	15.54
MWW	<i>P6/mmm</i>	—	—	—	—	—	—	0	2.409	2.256	0
NAB	<i>\bar{I}4m2</i>	—	—	1	—	0	—	0	—	1.162	0
NAT	<i>I4₁/amd</i>	—	—	1	—	0	—	0	—	4.572	0
NES	<i>Fmmm</i>	0	—	—	—	0	—	0.8871	—	2.787	8.078
NON	<i>Fmmm</i>	0	—	—	—	0	—	0.8899	—	3.772	6.713
NPO	<i>P\bar{6}2c</i>	—	—	—	—	0	0	—	—	4.574	0
NPT	<i>Pm\bar{3}m</i>	—	—	—	—	—	—	1.018	0	1.465	0
NSI	<i>C2/m</i>	—	—	—	—	0	—	—	—	5.065	0
OBW	<i>I4/mmm</i>	—	—	1	—	0	—	1.013	—	1.302	5.278
OFF	<i>P\bar{6}m2</i>	—	—	—	—	—	—	0	0	4.150	11.00
OKO	<i>C2/m</i>	—	—	—	—	0	—	—	—	3.579	12.44
OSI	<i>I4/mmm</i>	—	—	0	—	0	—	1.089	—	2.372	0
OSO	<i>P6₂22</i>	1	—	—	—	1.122	—	—	—	—	0
OWE	<i>Pmma</i>	—	—	—	—	0	—	0	—	6.306	8.861
PAU	<i>Im\bar{3}m</i>	—	—	0	—	1.644	—	0	0	0	14.14
PCR	<i>C2/m</i>	—	—	—	—	0	—	—	—	4.468	12.83
PHI	<i>Cmcm</i>	—	—	—	—	0	—	0	—	0	17.00
PON	<i>Pca2₁</i>	—	—	—	—	—	—	—	—	—	18.39
POS	<i>P4₂/mnm</i>	—	0	—	—	0	—	—	—	1.306	11.85
PSI	<i>Cmce</i>	—	—	—	—	0	—	—	—	0	20.45

Zeolite	Space group	TAD density									
		222	$\bar{4}$	$\bar{4}2m$	$\bar{4}3m$	2 (T nm ⁻¹)	3 (T nm ⁻¹)	2mm (T nm ⁻¹)	3m (T nm ⁻¹)	m (T nm ⁻²)	1 (T nm ⁻³)
PUN	<i>Pbcn</i>	—	—	—	—	1.165	—	—	—	—	13.44
RHO	<i>Im\bar{3}m</i>	—	—	0	—	1.915	—	0	0	0	0
RRO	<i>P2/c</i>	—	—	—	—	1.144	—	—	—	—	16.04
RSN	<i>Cmmm</i>	—	—	—	—	0	—	0.4816	—	2.709	0
RTE	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	17.58
RTH	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	16.43
RUT	<i>C2/m</i>	—	—	—	—	1.515	—	—	—	0	16.25
RWR	<i>I4₁/amd</i>	—	—	0	—	1.831	—	0	—	1.911	0
RWY	<i>Im\bar{3}m</i>	—	—	0	—	0	—	0	0	1.172	0
SAF	<i>Ibam</i>	0	—	—	—	0	—	—	—	0	19.12
SAO	<i>\bar{I}4m2</i>	—	—	0	—	1.043	—	0	—	0	12.14
SAS	<i>I4/mmm</i>	—	—	0	—	2.020	—	0	—	4.082	0
SAT	<i>R\bar{3}m</i>	—	—	—	—	0	—	—	0	0	16.90
SAV	<i>P4/nmm</i>	—	—	0	—	0	—	0	—	0	15.54
SBE	<i>I4/mmm</i>	—	—	0	—	0	—	0	—	0	13.97
SBN	<i>P6₃/mmc</i>	—	—	—	—	0	—	0.8060	2.911	0	0
SBS	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	0	13.90
SBT	<i>R\bar{3}m</i>	—	—	—	—	0	—	0	0	0	13.90
SEW	<i>Pmmn</i>	—	—	—	—	—	—	0.7020	—	2.457	12.12
SFE	<i>P2₁/m</i>	—	—	—	—	—	—	—	—	4.536	0
SFF	<i>P2₁/m</i>	—	—	—	—	—	—	—	—	0	17.65
SFG	<i>Pmma</i>	—	—	—	—	0	—	0.7725	—	2.485	13.71
SFH	<i>Cmcm</i>	—	—	—	—	0	—	0	—	4.374	0
SFN	<i>C2/m</i>	—	—	—	—	0	—	—	—	4.375	0
SFO	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	15.49
SFS	<i>P2₁/m</i>	—	—	—	—	—	—	—	—	0	16.94
SFV	<i>P\bar{4}m2</i>	—	—	0	—	1.413	—	0	—	0	17.64
SFW	<i>R\bar{3}m</i>	—	—	—	—	0	—	—	0	0	15.61
SGT	<i>I4₁/amd</i>	—	—	0	—	1.962	—	0	—	3.435	0
SIV	<i>Cmcm</i>	—	—	—	—	0	—	0	—	0	17.06
SOD	<i>Im\bar{3}m</i>	—	—	1	—	0	—	0	0	0	0
SOF	<i>C2/c</i>	—	—	—	—	0	—	—	—	—	16.75
SOS	<i>Pmna</i>	—	—	—	—	0	—	—	—	0	17.19
SSF	<i>P6/mmm</i>	—	—	—	—	—	—	1.171	0	3.744	7.594
SSY	<i>Pmmn</i>	—	—	—	—	—	—	0.7198	—	3.883	0
STF	<i>C2/m</i>	—	—	—	—	0	—	—	—	3.939	12.89
STI	<i>Fmmm</i>	1	—	—	—	0	—	0	—	6.676	7.630
STO	<i>P2/m</i>	—	—	—	—	0	—	—	—	0	18.72
STT	<i>P2₁/c</i>	—	—	—	—	—	—	—	—	—	16.91
STW	<i>P6₁22</i>	—	—	—	—	0	—	—	—	—	16.46
SVV	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	17.99
SWY	<i>P6₃/mmc</i>	—	—	—	—	0	—	0	0	0	16.51
SZR	<i>Cmmm</i>	—	—	—	—	0	—	1.076	—	3.027	8.119
TER	<i>Cmcm</i>	—	—	—	—	0	—	0	—	5.129	7.078
THO	<i>Pmma</i>	—	—	—	—	0	—	1.573	—	4.577	0
TOL	<i>P\bar{3}m1</i>	—	—	—	—	1.617	—	0	0	0	14.65
TON	<i>Cmcm</i>	—	—	—	—	0	—	1.136	—	3.266	0
TSC	<i>Fm\bar{3}m</i>	—	—	—	0	—	—	0	0	0	13.55
TUN	<i>C2/m</i>	—	—	—	—	0	—	—	—	0	17.79
UEI	<i>Fmm2</i>	—	—	—	—	0	—	0	—	0	18.54
UFI	<i>I4/mmm</i>	—	—	0	—	0	—	0	—	2.346	7.716
UOS	<i>Pmma</i>	—	—	—	—	0	—	0	—	4.542	11.99
UOV	<i>Amm2</i>	—	—	—	—	—	—	0	—	2.819	14.24

Zeolite	Space group	TAD density									
		222	$\bar{4}$	$\bar{4}2m$	$\bar{4}3m$	2 (T nm ⁻¹)	3 (T nm ⁻¹)	2mm (T nm ⁻¹)	3m (T nm ⁻¹)	m (T nm ⁻²)	1 (T nm ⁻³)
UOZ	<i>P4/nnc</i>	1	1	–	–	0	–	–	–	–	15.65
USI	<i>C2/m</i>	–	–	–	–	0	–	–	–	0	16.03
UTL	<i>C2/m</i>	–	–	–	–	0	–	–	–	2.886	11.63
UWY	<i>Pmmm</i>	–	–	–	–	–	–	0	–	2.801	11.12
VET	<i>P$\bar{4}$</i>	–	1	–	–	0	–	–	–	–	19.03
VFI	<i>P6₃/mcm</i>	–	–	–	–	0	0	0	0	2.562	9.646
VNI	<i>P4₂/ncm</i>	0	0	–	–	0	–	0.5892	–	4.197	4.784
VSV	<i>I4₁/amd</i>	–	–	1	–	0	–	0	–	2.703	0
WEI	<i>Cccm</i>	1	–	–	–	0	–	–	–	0	12.97
YUG	<i>C2/m</i>	–	–	–	–	0	–	–	–	0	18.58
ZON	<i>Pbcm</i>	–	–	–	–	0	–	–	–	0	17.92

Table S2 Occurrence and TAD density for the site symmetries occurring in 84 292 hypothetical zeolite structures.

Site symmetry	Occurrence	Highest TAD density
$\bar{4}_2m$	1	1
2	1088	1.621 T nm ⁻¹
m	1888	4.556 T nm ⁻²
1	84289	17.97 T nm ⁻³

Table S3 Numbers of WP combinations for 12 space groups.

Space group	Unit cell			Numbers of WP combinations				Total decrease in WP combinations / times
	$a = b$ / nm	c / nm	volume / nm ³	All WPs	Prohibited WPs removed	Prohibited WPs removed; rotation axes restricted	Prohibited WPs removed; rotation axes and mirror planes restricted	
<i>P4</i>	1.0	1.0	1.00	1222	24	9	9	135.8
	1.0	1.3	1.30	2715	30	9	9	301.7
	1.0	1.6	1.60	5378	48	16	16	336.1
	1.0	1.9	1.90	10625	70	20	20	531.3
	1.0	2.2	2.20	17450	85	27	27	646.3
	1.3	1.0	1.69	6838	56	13	13	526.0
	1.3	1.3	2.20	17450	85	16	16	1090.6
	1.3	1.6	2.70	37240	133	28	28	1330.0
	1.3	1.9	3.21	70388	176	32	32	2199.6
	1.3	2.2	3.72	121875	242	47	47	2593.1
	1.6	1.0	2.56	31881	120	19	19	1677.9
	1.6	1.3	3.33	79988	184	24	24	3332.8
	1.6	1.6	4.10	178365	280	40	40	4459.1
	1.6	1.9	4.86	347688	396	48	48	7243.5
	1.6	2.2	5.63	613431	532	70	70	8763.3
	1.9	1.0	3.61	108645	225	27	27	4023.9
	1.9	1.3	4.69	303688	384	36	36	8435.8
	1.9	1.6	5.78	661141	546	56	56	11806.1
	1.9	1.9	6.86	1314613	782	68	68	19332.5
	1.9	2.2	7.94	2289974	1060	100	100	22899.7
	2.2	1.0	4.84	347688	396	36	36	9658.0
	2.2	1.3	6.29	946172	659	47	47	20131.3
	2.2	1.6	7.74	2111702	1004	78	78	27073.1
	2.2	1.9	9.20	4109847	1403	92	92	44672.3
	2.2	2.2	10.65	7272269	1868	132	132	55092.9
<i>I4/mmm</i>	1.0	1.0	1.00	241	22	5	4	60.3
	1.0	1.3	1.30	487	32	7	5	97.4
	1.0	1.6	1.60	1367	100	12	8	170.9
	1.0	1.9	1.90	3321	186	19	12	276.8
	1.0	2.2	2.20	5664	258	23	14	404.6
	1.3	1.0	1.69	1859	100	32	32	58.1
	1.3	1.3	2.20	5664	258	58	56	101.1
	1.3	1.6	2.70	19036	962	134	119	160.0
	1.3	1.9	3.21	44680	1944	204	174	256.8
	1.3	2.2	3.72	116978	3740	301	244	479.4
	1.6	1.0	2.56	15068	604	138	130	115.9
	1.6	1.3	3.33	54424	1944	295	285	191.0
	1.6	1.6	4.10	198550	6806	645	605	328.2
	1.6	1.9	4.86	614436	15200	1070	956	642.7
	1.6	2.2	5.63	1681908	41076	1912	1630	1031.8
	1.9	1.0	3.61	97170	3740	571	553	175.7
	1.9	1.3	4.69	528364	15200	1404	1354	390.2
	1.9	1.6	5.78	1922492	41076	2552	2334	823.7
	1.9	1.9	6.86	6751048	125664	4900	4335	1557.3
	1.9	2.2	7.94	20457983	326470	8500	7220	2833.5
	2.2	1.0	4.84	614436	15200	1404	1270	483.8
	2.2	1.3	6.29	3679976	82512	3840	3422	1075.4

Space group	Unit cell			Numbers of WP combinations				Total decrease in WP combinations / times
	$a = b$ / nm	c / nm	volume / nm ³	All WPs	Prohibited WPs removed	Prohibited WPs removed; rotation axes restricted	Prohibited WPs removed; rotation axes and mirror planes restricted	
$I4_1/acd$	2.2	1.6	7.74	16558561	274990	7645	6786	2440.1
	2.2	1.9	9.20	60695900	921602	15057	12687	4784.1
	2.2	2.2	10.65	190691682	2330250	24852	19028	10021.6
	1.0	1.0	1.00	7	6	5	5	1.4
	1.0	1.3	1.30	5	4	3	3	1.7
	1.0	1.6	1.60	13	10	7	7	1.9
	1.0	1.9	1.90	27	20	11	11	2.5
	1.0	2.2	2.20	22	16	13	13	1.7
	1.3	1.0	1.69	13	10	7	7	1.9
	1.3	1.3	2.20	22	16	8	8	2.8
	1.3	1.6	2.70	72	50	16	16	4.5
	1.3	1.9	3.21	104	70	16	16	6.5
	1.3	2.2	3.72	159	105	39	39	4.1
	1.6	1.0	2.56	42	30	15	15	2.8
	1.6	1.3	3.33	104	70	23	23	4.5
	1.6	1.6	4.10	215	139	30	30	7.2
	1.6	1.9	4.86	306	195	36	36	8.5
	1.6	2.2	5.63	538	333	83	83	6.5
	1.9	1.0	3.61	159	105	29	29	5.5
	1.9	1.3	4.69	306	195	36	36	8.5
$P3$	1.9	1.6	5.78	538	333	42	42	12.8
	1.9	1.9	6.86	1120	673	54	54	20.7
	1.9	2.2	7.94	1695	1002	120	120	14.1
	2.2	1.0	4.84	306	195	62	62	4.9
	2.2	1.3	6.29	880	533	93	93	9.5
	2.2	1.6	7.74	1695	1002	119	119	14.2
	2.2	1.9	9.20	2901	1679	132	132	22.0
	2.2	2.2	10.65	4760	2715	312	312	15.3
	1.0	1.0	0.87	1491	1491	81	81	18.4
	1.0	1.3	1.13	3861	3861	234	234	16.5
	1.0	1.6	1.39	7280	7280	278	278	26.2
	1.0	1.9	1.65	14395	14395	667	667	21.6
	1.0	2.2	1.91	25743	25743	1368	1368	18.8
	1.3	1.0	1.46	9845	9845	135	135	72.9
	1.3	1.3	1.90	25743	25743	405	405	63.6
	1.3	1.6	2.34	56414	56414	512	512	110.2
	1.3	1.9	2.78	107712	107712	1167	1167	92.3
	1.3	2.2	3.22	176655	176655	2304	2304	76.7
	1.6	1.0	2.22	42735	42735	198	198	215.8
	1.6	1.3	2.88	115479	115479	598	598	193.1
	1.6	1.6	3.55	257631	257631	747	747	344.9
	1.6	1.9	4.21	502320	502320	1750	1750	287.0
	1.6	2.2	4.88	885780	885780	3456	3456	256.3
	1.9	1.0	3.13	164665	164665	279	279	590.2
	1.9	1.3	4.06	453205	453205	875	875	517.9
	1.9	1.6	5.00	1011136	1011136	1067	1067	947.6
	1.9	1.9	5.94	1905569	1905569	2458	2458	775.3
	1.9	2.2	6.88	3392756	3392756	4896	4896	693.0
	2.2	1.0	4.19	502320	502320	378	378	1328.9

Space group	Unit cell			Numbers of WP combinations				Total decrease in WP combinations / times
	$a = b$ / nm	c / nm	volume / nm ³	All WPs	Prohibited WPs removed	Prohibited WPs removed; rotation axes restricted	Prohibited WPs removed; rotation axes and mirror planes restricted	
$R\bar{3}m$	2.2	1.3	5.45	1408446	1408446	1173	1173	1200.7
	2.2	1.6	6.71	3088365	3088365	1430	1430	2159.7
	2.2	1.9	7.96	6124460	6124460	3334	3334	1837.0
	2.2	2.2	9.22	10718396	10718396	6624	6624	1618.1
	1.0	1.0	0.87	16	1	0	0	–
	1.0	1.3	1.13	22	5	3	3	7.3
	1.0	1.6	1.39	50	9	7	7	7.1
	1.0	1.9	1.65	64	8	6	6	10.7
	1.0	2.2	1.91	110	12	10	10	11.0
	1.3	1.0	1.46	50	9	6	6	8.3
	1.3	1.3	1.90	110	12	6	6	18.3
	1.3	1.6	2.34	228	30	16	16	14.3
	1.3	1.9	2.78	348	41	21	21	16.6
	1.3	2.2	3.22	616	61	33	33	18.7
	1.6	1.0	2.22	192	23	11	11	17.5
	1.6	1.3	2.88	422	41	13	13	32.5
	1.6	1.6	3.55	850	85	32	32	26.6
	1.6	1.9	4.21	1567	151	45	45	34.8
	1.6	2.2	4.88	2649	232	70	70	37.8
	1.9	1.0	3.13	502	61	17	17	29.5
$R\bar{3}c$	1.9	1.3	4.06	1357	151	33	33	41.1
	1.9	1.6	5.00	3029	312	69	69	43.9
	1.9	1.9	5.94	5443	461	86	86	63.3
	1.9	2.2	6.88	10057	816	140	140	71.8
	2.2	1.0	4.19	1567	151	52	52	30.1
	2.2	1.3	5.45	3855	381	94	94	41.0
	2.2	1.6	6.71	9211	840	216	216	42.6
	2.2	1.9	7.96	17349	1392	281	281	61.7
	2.2	2.2	9.22	33341	2627	518	518	64.4
	1.0	1.0	0.87	2	1	0	0	–
	1.0	1.3	1.13	6	2	1	1	6.0
	1.0	1.6	1.39	12	3	1	1	12.0
	1.0	1.9	1.65	10	2	1	1	10.0
	1.0	2.2	1.91	16	3	2	2	8.0
	1.3	1.0	1.46	12	3	1	1	12.0
	1.3	1.3	1.90	16	3	1	1	16.0
	1.3	1.6	2.34	33	6	2	2	16.5
	1.3	1.9	2.78	45	9	5	5	9.0
	1.3	2.2	3.22	55	11	6	6	9.2
	1.6	1.0	2.22	25	6	3	3	8.3
	1.6	1.3	2.88	45	9	2	2	22.5
	1.6	1.6	3.55	75	14	4	4	18.8
	1.6	1.9	4.21	114	22	10	10	11.4
	1.6	2.2	4.88	165	28	10	10	16.5
	1.9	1.0	3.13	55	11	4	4	13.8
	1.9	1.3	4.06	114	22	6	6	19.0
	1.9	1.6	5.00	201	34	6	6	33.5
	1.9	1.9	5.94	273	45	14	14	19.5
	1.9	2.2	6.88	406	65	14	14	29.0

Space group	Unit cell			Numbers of WP combinations				Total decrease in WP combinations / times
	$a = b$ / nm	c / nm	volume / nm ³	All WPs	Prohibited WPs removed	Prohibited WPs removed; rotation axes restricted	Prohibited WPs removed; rotation axes and mirror planes restricted	
<i>P6</i>	2.2	1.0	4.19	114	22	7	7	16.3
	2.2	1.3	5.45	231	39	7	7	33.0
	2.2	1.6	6.71	422	68	10	10	42.2
	2.2	1.9	7.96	594	92	22	22	27.0
	2.2	2.2	9.22	910	138	25	25	36.4
	1.0	1.0	0.87	210	34	13	13	16.2
	1.0	1.3	1.13	490	65	22	22	22.3
	1.0	1.6	1.39	876	104	36	36	24.3
	1.0	1.9	1.65	1644	165	54	54	30.4
	1.0	2.2	1.91	2832	252	95	95	29.8
	1.3	1.0	1.46	1161	129	23	23	50.5
	1.3	1.3	1.90	2832	252	38	38	74.5
	1.3	1.6	2.34	5936	448	64	64	92.8
	1.3	1.9	2.78	10960	710	94	94	116.6
	1.3	2.2	3.22	17590	1020	160	160	109.9
	1.6	1.0	2.22	4564	366	33	33	138.3
	1.6	1.3	2.88	11705	745	57	57	205.4
	1.6	1.6	3.55	25257	1338	94	94	268.7
	1.6	1.9	4.21	48097	2184	140	140	343.6
	1.6	2.2	4.88	83300	3300	240	240	347.1
	1.9	1.0	3.13	16435	965	47	47	349.7
	1.9	1.3	4.06	43547	2023	82	82	531.1
	1.9	1.6	5.00	94748	3648	134	134	707.1
	1.9	1.9	5.94	175626	5814	196	196	896.1
<i>P6₃/mcm</i>	1.9	2.2	6.88	308572	8888	340	340	907.6
	2.2	1.0	4.19	48097	2184	63	63	763.4
	2.2	1.3	5.45	130824	4662	110	110	1189.3
	2.2	1.6	6.71	130824	8316	180	180	726.8
	2.2	1.9	7.96	550638	13782	266	266	2070.1
	2.2	2.2	9.22	954338	20867	400	400	2385.8
	1.0	1.0	0.87	99	11	3	3	33.0
	1.0	1.3	1.13	327	33	6	6	54.5
	1.0	1.6	1.39	628	62	18	18	34.9
	1.0	1.9	1.65	1121	94	32	32	35.0
	1.0	2.2	1.91	2483	181	52	52	47.8
	1.3	1.0	1.46	858	73	13	13	66.0
	1.3	1.3	1.90	2483	181	20	20	124.2
	1.3	1.6	2.34	6174	420	87	87	71.0
	1.3	1.9	2.78	13664	860	221	221	61.8
	1.3	2.2	3.22	23513	1446	300	300	78.4
	1.6	1.0	2.22	3982	280	39	38	104.8
	1.6	1.3	2.88	13664	860	79	78	175.2
	1.6	1.6	3.55	38489	2211	222	221	174.2
	1.6	1.9	4.21	94779	5105	684	683	138.8
	1.6	2.2	4.88	208512	10662	1056	1054	197.8
	1.9	1.0	3.13	23513	1446	118	114	206.3
	1.9	1.3	4.06	82103	4580	286	274	299.6
	1.9	1.6	5.00	266080	13405	980	961	276.9
	1.9	1.9	5.94	653379	31170	2790	2757	237.0

Space group	Unit cell			Numbers of WP combinations				Total decrease in WP combinations / times
	$a = b$ / nm	c / nm	volume / nm ³	All WPs	Prohibited WPs removed	Prohibited WPs removed; rotation axes restricted	Prohibited WPs removed; rotation axes and mirror planes restricted	
$P6_3/mmc$	1.9	2.2	6.88	1441319	65995	4368	4311	334.3
	2.2	1.0	4.19	94779	5105	286	260	364.5
	2.2	1.3	5.45	423917	20765	650	580	730.9
	2.2	1.6	6.71	1313693	61134	2350	2190	599.9
	2.2	1.9	7.96	3466540	152105	6978	6668	519.9
	2.2	2.2	9.22	8114722	345520	11022	10406	779.8
	1.0	1.0	0.87	193	16	5	4	48.3
	1.0	1.3	1.13	641	52	12	9	71.2
	1.0	1.6	1.39	1228	97	46	33	37.2
	1.0	1.9	1.65	2219	157	65	43	51.6
	1.0	2.2	1.91	4921	304	119	75	65.6
	1.3	1.0	1.46	1688	115	25	24	70.3
	1.3	1.3	1.90	4921	304	48	44	111.8
	1.3	1.6	2.34	12228	707	204	176	69.5
	1.3	1.9	2.78	27138	1466	325	260	104.4
	1.3	2.2	3.22	46759	2506	549	420	111.3
	1.6	1.0	2.22	7884	463	65	64	123.2
	1.6	1.3	2.88	27138	1466	139	131	207.2
	1.6	1.6	3.55	76585	3850	655	589	130.0
	1.6	1.9	4.21	188817	9034	1121	937	201.5
	1.6	2.2	4.88	415728	19104	2180	1705	243.8
	1.9	1.0	3.13	46759	2506	706	619	75.5
	1.9	1.3	4.06	163465	8092	458	428	381.9
	1.9	1.6	5.00	530464	24106	2213	1957	271.1
	1.9	1.9	5.94	1304025	56835	3660	3004	434.1
$P23$	1.9	2.2	6.88	2877511	121232	7053	5401	532.8
	2.2	1.0	4.19	188817	9034	600	592	318.9
	2.2	1.3	5.45	845691	37567	1441	1354	624.6
	2.2	1.6	6.71	2622167	112180	7704	6817	384.7
	2.2	1.9	7.96	6923984	282392	13090	10693	647.5
	2.2	2.2	9.22	16211758	646138	26545	20060	808.2
	1.0	1.0	1.00	415	133	121	121	3.4
	1.3	1.3	2.20	8986	2560	1234	1234	7.3
	1.6	1.6	4.10	172858	46292	9420	9420	18.4
	1.9	1.9	6.86	2547625	666215	23039	23039	110.6
	2.2	2.2	10.65	27937296	7169724	68937	68937	405.3
$Im\bar{3}m$	1.0	1.0	1.00	13	2	2	2	6.5
	1.3	1.3	2.20	74	6	5	5	14.8
	1.6	1.6	4.10	540	44	33	33	16.4
	1.9	1.9	6.86	4477	239	161	161	27.8
$Ia\bar{3}d$	2.2	2.2	10.65	35550	1363	603	603	59.0
	1.0	1.0	1.00	2	0	0	0	–
	1.3	1.3	2.20	4	3	2	2	2.0
	1.6	1.6	4.10	29	10	4	4	7.3
	1.9	1.9	6.86	106	36	9	9	11.8
	2.2	2.2	10.65	356	106	26	26	13.7

Table S4 320 optimized hypothetical zeolite frameworks built from 804 WP combinations in space group $Im\bar{3}m$.

hypothetical structure	number of unique T atoms	WP combinations	Framework density /T nm ⁻³	<i>a</i> / nm
H229d1(SOD)	1	<i>d</i>	17.41	0.8834
H229f2(ACO)	1	<i>f</i>	16.99	0.9802
H229dh3	2	<i>dh</i>	8.798	1.599
H229dfh4	3	<i>dfh</i>	19.08	1.397
H229i5(RHO)	1	<i>i</i>	14.89	1.477
H229fk6	2	<i>fk</i>	13.91	1.663
H229dj7	2	<i>dj</i>	20.28	1.436
H229dffh8	4	<i>dffh</i>	20.66	1.488
H229fhhj9	4	<i>fhhj</i>	18.86	1.811
H229ij10	2	<i>ij</i>	14.81	1.865
H229gjk11	3	<i>gjk</i>	13.20	2.087
H229dfhj12	4	<i>dfhj</i>	19.81	1.716
H229gkk13	3	<i>gkk</i>	12.56	2.122
H229fik14	3	<i>fik</i>	15.91	1.916
H229ik15	2	<i>ik</i>	18.10	1.744
H229hij16	3	<i>hij</i>	18.12	1.878
H229dj17	3	<i>djk</i>	20.13	1.751
H229fghj18	4	<i>fghj</i>	18.77	1.814
H229l19	1	<i>l</i>	15.47	1.838
H229kk20	2	<i>kk</i>	16.65	1.793
H229fghk21	4	<i>fghk</i>	14.42	1.980
H229dhhi22	4	<i>dhhi</i>	18.92	1.787
H229djj23	3	<i>djj</i>	16.86	1.857
H229j24(RWY)	1	<i>j</i>	7.613	1.847
H229fk25	2	<i>fk</i>	13.91	1.663
H229ffhj26	4	<i>ffhj</i>	16.92	1.832
H229fhj27	3	<i>fhj</i>	17.31	1.720
H229jj28	2	<i>jj</i>	17.88	1.751
H229hjj29	3	<i>hjj</i>	22.89	1.737
H229hj30	2	<i>hj</i>	9.238	1.983
H229jk31	2	<i>jk</i>	13.13	1.941
H229hkk32	3	<i>hkk</i>	19.16	1.843
H229ffhk33	4	<i>ffhk</i>	13.55	1.973
H229fhk34	3	<i>fhk</i>	19.86	1.642
H229fjk35	3	<i>fjk</i>	13.92	2.004
H229hjj36	3	<i>hjj</i>	20.31	1.808
H229hk37	2	<i>hk</i>	13.98	1.727
H229dffhk38	5	<i>dffhk</i>	16.13	1.930
H229dhk39	3	<i>dhk</i>	14.47	1.797
H229fhhk40	4	<i>fhhk</i>	21.02	1.747
H229dfhj41	5	<i>dfhj</i>	20.49	1.782
H229hhi42	3	<i>hhi</i>	16.79	1.788
H229gj43	2	<i>gj</i>	9.271	1.980
H229fhhk44	4	<i>fhhk</i>	20.06	1.774
H229fhk45	3	<i>fhk</i>	16.89	1.734
H229fhj46	4	<i>fhj</i>	18.86	1.811
H229gi47	2	<i>gi</i>	18.43	1.575
H229dfhk48	4	<i>dfhk</i>	17.66	1.782
H229gik49	3	<i>gik</i>	17.75	1.891
H229dij50	3	<i>dij</i>	12.62	2.045
H229kk51	2	<i>kk</i>	17.07	1.778
H229hi52	2	<i>hi</i>	8.308	2.054
H229hjj53	3	<i>hjj</i>	14.89	2.005
H229ghi54	3	<i>ghi</i>	13.19	1.938
H229hij55	3	<i>hij</i>	19.88	1.821
H229ffk56	3	<i>ffk</i>	15.13	1.742
H229fkk57	3	<i>fkk</i>	17.89	1.843
H229fghj58	4	<i>fghj</i>	19.47	1.792
H229gl59	2	<i>gl</i>	16.72	1.929
H229ffhhik60	6	<i>ffhhik</i>	16.99	2.180
H229hjjk61	4	<i>hjjk</i>	18.14	2.100
H229fhjjk62	5	<i>fhjjk</i>	16.33	2.242
H229fhikk63	5	<i>fhikk</i>	21.63	2.041

hypothetical structure	number of unique T atoms	WP combinations	Framework density /T nm ⁻³	<i>a</i> / nm
H229fhjjk64	5	<i>fhijk</i>	16.63	2.228
H229ijk65	3	<i>ijk</i>	17.08	2.035
H229ijj66	3	<i>ijj</i>	17.05	2.037
H229kkk67	3	<i>kkk</i>	12.30	2.271
H229ffgjk68	5	<i>ffgjk</i>	18.26	2.026
H229fhjkk69	5	<i>fhjkk</i>	27.05	1.895
H229jkk70	3	<i>jkk</i>	12.27	2.273
H229ijk71	3	<i>ijk</i>	19.24	1.956
H229ffhij72	5	<i>ffhij</i>	16.98	2.076
H229ffhjj73	5	<i>ffhjj</i>	16.82	2.083
H229fjk74	3	<i>fjk</i>	11.29	2.149
H229fhjkk75	5	<i>fhjkk</i>	16.28	2.244
H229dffhij76	6	<i>dffhij</i>	17.66	2.102
H229fhjkk77	5	<i>fhjkk</i>	15.50	2.281
H229fijk78	4	<i>fijk</i>	16.41	2.136
H229fgikk79	5	<i>fgikk</i>	17.92	2.174
H229hhjj80	4	<i>hhjj</i>	20.69	1.909
H229dhjj81	4	<i>dhjj</i>	15.48	2.043
H229ffghjk82	6	<i>ffghjk</i>	16.15	2.217
H229hhjk83	4	<i>hhjk</i>	13.51	2.201
H229djkk84	4	<i>djkk</i>	14.50	2.207
H229hjkk85	4	<i>hjkk</i>	16.48	2.168
H229ghjj86	4	<i>ghjj</i>	16.98	2.039
H229ghl87	3	<i>ghl</i>	10.14	2.422
H229fghjk88	5	<i>fghjk</i>	19.79	2.007
H229fhjjk89	5	<i>fhjjk</i>	12.01	2.484
H229ffgkk90	5	<i>ffgkk</i>	16.17	2.110
H229fjkk91	4	<i>fjkk</i>	15.03	2.200
H229dffjkk92	6	<i>dffjkk</i>	19.95	2.112
H229hil93	3	<i>hil</i>	18.52	2.085
H229ghhjk94	5	<i>ghhjk</i>	16.02	2.189
H229fgjkk95	5	<i>fgjkk</i>	20.59	2.075
H229hijj96	4	<i>hijj</i>	18.93	2.070
H229fgijk97	5	<i>fgijk</i>	17.61	2.186
H229fhkkk98	5	<i>fhkkk</i>	16.31	2.243
H229gl99	2	<i>gl</i>	9.060	2.366
H229dhjjk100	5	<i>dhjjk</i>	16.81	2.204
H229fhjjk101	5	<i>fhjjk</i>	16.94	2.215
H229gil102	3	<i>gil</i>	14.12	2.283
H229gik103	3	<i>gik</i>	12.84	2.106
H229dhhjk104	5	<i>dhhjk</i>	14.29	2.218
H229ghhkk105	5	<i>ghhkk</i>	16.89	2.150
H229ikk106	3	<i>ikk</i>	10.94	2.361
H229ffkl107	4	<i>ffkl</i>	20.03	2.064
H229fhkk108	4	<i>fhkk</i>	10.94	2.317
H229hijk109	4	<i>hijk</i>	13.51	2.317
H229dfjjk110	5	<i>dfjjk</i>	17.90	2.126
H229fhjjk111	5	<i>fhjjk</i>	13.03	2.417
H229ffhkk112	5	<i>ffhkk</i>	16.83	2.083
H229fhjjk113	5	<i>fhjjk</i>	20.73	2.071
H229ffhjk114	5	<i>ffhjk</i>	16.82	2.083
H229dffijk115	6	<i>dffijk</i>	17.52	2.206
H229hijk116	4	<i>hijk</i>	16.05	2.188
H229fkkk117	4	<i>fkkk</i>	11.48	2.407
H229ghkk118	4	<i>ghkk</i>	17.42	2.022
H229fkkk119	5	<i>fkkk</i>	15.94	2.227
H229fgkkk120	5	<i>fgkkk</i>	20.10	2.092
H229fhijk121	5	<i>fhijk</i>	17.71	2.182
H229ffghij122	6	<i>ffghij</i>	15.52	2.246
H229ffhijk123	6	<i>ffhijk</i>	20.45	2.049
H229dijk124	4	<i>dijk</i>	12.19	2.339
H229ffhijk125	6	<i>ffhijk</i>	15.31	2.257
H229jjk126	3	<i>jjk</i>	19.17	1.958
H229ffghjk127	6	<i>ffghjk</i>	19.44	2.084
H229hkk128	3	<i>hkk</i>	12.94	2.101

hypothetical structure	number of unique T atoms	WP combinations	Framework density /T nm ⁻³	<i>a</i> / nm
H229ffjkk129	5	<i>ffjkk</i>	17.99	2.139
H229fik130	3	<i>fik</i>	14.71	1.967
H229ffghik131	6	<i>ffghik</i>	18.92	2.103
H229dfhjk132	5	<i>dfhjk</i>	17.91	2.022
H229ffkk133	4	<i>ffkk</i>	16.09	1.996
H229dffjkk134	6	<i>dffjkk</i>	17.16	2.221
H229dhjl135	4	<i>dhjl</i>	18.26	2.144
H229ffhhjj136	6	<i>ffhhjj</i>	18.06	2.136
H229ffghk137	5	<i>ffghk</i>	17.56	1.939
H229fgkk138	4	<i>fgkk</i>	12.62	2.209
H229gjl139	3	<i>gjl</i>	15.17	2.229
H229dhjjj140	5	<i>dhjjj</i>	17.20	2.187
H229fghjk141	5	<i>fghjk</i>	12.91	2.314
H229ghhjk142	5	<i>ghhjk</i>	18.00	2.105
H229hhjj143	4	<i>hhjj</i>	16.57	2.056
H229fghk144	4	<i>fghk</i>	14.16	1.993
H229fhjk145	4	<i>fhjk</i>	14.30	2.118
H229fhhjk146	5	<i>fhhjk</i>	13.58	2.275
H229ghik147	4	<i>ghik</i>	16.34	2.065
H229hjk148	3	<i>hjk</i>	12.90	2.103
H229hjl149	3	<i>hjl</i>	16.78	2.155
H229gijk150	4	<i>gijk</i>	13.46	2.320
H229fhjjk151	5	<i>fhjjk</i>	16.00	2.257
H229jjj152	3	<i>jjj</i>	13.72	2.190
H229fgikk153	5	<i>fgikk</i>	18.52	2.150
H229hij154	3	<i>hij</i>	15.03	1.999
H229dffhij155	6	<i>dffhij</i>	20.84	1.989
H229djkl156	3	<i>djk</i>	13.40	2.005
H229gijk157	4	<i>gijk</i>	16.95	2.148
H229hjjk158	4	<i>hjjk</i>	18.18	2.098
H229fikk159	4	<i>fikk</i>	18.81	2.041
H229ghhjj160	5	<i>ghhjj</i>	17.09	2.142
H229ffhik161	5	<i>ffhik</i>	18.39	2.022
H229fghjk162	5	<i>fghjk</i>	16.16	2.147
H229ffikk163	5	<i>ffikk</i>	15.45	2.250
H229ffhik164	5	<i>ffhik</i>	17.75	2.046
H229gijk165	4	<i>gijk</i>	16.86	2.152
H229fghhkk166	6	<i>fghhkk</i>	20.74	2.070
H229fjkk167	4	<i>fjkk</i>	18.76	2.043
H229hl168	2	<i>hl</i>	10.95	2.221
H229dijk169	4	<i>dijk</i>	18.46	2.037
H229hij170	3	<i>hij</i>	13.98	2.047
H229ffghij171	6	<i>ffghij</i>	23.15	1.966
H229gjij172	4	<i>gjij</i>	19.94	2.035
H229ffhkk173	5	<i>ffhkk</i>	17.28	2.064
H229gijk174	4	<i>gijk</i>	14.44	2.266
H229ffhhkk175	6	<i>ffhhkk</i>	15.84	2.231
H229ffghk176	5	<i>ffghk</i>	17.01	1.960
H229dhjk177	4	<i>dhjk</i>	13.35	2.146
H229dhjjk178	5	<i>dhjjk</i>	17.45	2.177
H229fhjjk179	5	<i>fhjjk</i>	22.85	2.004
H229ffjkk180	5	<i>ffjkk</i>	19.10	2.096
H229kkk181	3	<i>kkk</i>	16.33	2.066
H229hkk182	3	<i>hkk</i>	14.44	2.026
H229fhkk183	4	<i>fhkk</i>	14.06	2.131
H229jl184	2	<i>jl</i>	15.23	2.115
H229dijk185	4	<i>dijk</i>	17.07	2.091
H229fgjjk186	5	<i>fgjjk</i>	20.23	2.088
H229gikk187	4	<i>gikk</i>	17.20	2.137
H229ffjkk188	5	<i>ffjkk</i>	19.44	2.084
H229hkl189	3	<i>hkl</i>	17.81	2.113
H229ffikk190	5	<i>ffikk</i>	16.51	2.201
H229fhjkk191	5	<i>fhjkk</i>	17.77	2.180
H229ffijk192	5	<i>ffijk</i>	18.46	2.120
H229fhhkk193	5	<i>fhhkk</i>	15.34	2.185

hypothetical structure	number of unique T atoms	WP combinations	Framework density /T nm ⁻³	<i>a</i> / nm
H229fjkk194	4	<i>fjkk</i>	17.10	2.107
H229fkl195	3	<i>fkl</i>	12.93	2.313
H229fgkl196	4	<i>fgkl</i>	20.52	2.078
H229hjjk197	4	<i>hjjk</i>	17.01	2.146
H229ghkk198	4	<i>ghkk</i>	13.48	2.202
H229kl199	2	<i>kl</i>	14.19	2.165
H229fhikk200	5	<i>fhikk</i>	18.58	2.147
H229dfjkk201	5	<i>dfjkk</i>	15.13	2.248
H229fhjkk202	5	<i>fhjkk</i>	19.76	2.104
H229djkk203	4	<i>djkk</i>	20.50	1.967
H229gkl204	3	<i>gkl</i>	19.23	2.060
H229fhijk205	5	<i>fhijk</i>	17.37	2.196
H229fhjjk206	5	<i>fhjjk</i>	15.57	2.278
H229ghhkk207	5	<i>ghhkk</i>	22.39	1.958
H229hhij208	4	<i>hhij</i>	12.38	2.266
H229hik209	3	<i>hik</i>	9.838	2.302
H229dffjk210	5	<i>dffjk</i>	14.93	2.109
H229fhjjk211	5	<i>fhjjk</i>	20.70	2.071
H229ghjk212	4	<i>ghjk</i>	18.25	1.991
H229dffjjk213	6	<i>dffjjk</i>	19.85	2.116
H229ffik214	4	<i>ffik</i>	13.01	2.143
H229dffhjk215	6	<i>dffhjk</i>	20.36	2.004
H229fghhik216	6	<i>fghhik</i>	12.74	2.435
H229ghjk217	4	<i>ghjk</i>	16.06	2.077
H229hikk218	4	<i>hikk</i>	12.72	2.364
H229fgijk219	5	<i>fgijk</i>	16.61	2.229
H229ffghkk220	6	<i>ffghkk</i>	17.96	2.140
H229fhkkk221	5	<i>fhkkk</i>	14.00	2.360
H229jl222	2	<i>jl</i>	12.25	2.274
H229fhjkk223	5	<i>fhjkk</i>	20.07	2.093
H229ffkkk224	5	<i>ffkkk</i>	19.03	2.099
H229ijk225	3	<i>ijk</i>	15.07	2.122
H229dfijk226	5	<i>dfijk</i>	19.48	2.067
H229hkk227	3	<i>hkk</i>	10.93	2.223
H229il228	2	<i>il</i>	14.16	2.167
H229hijk229	4	<i>hijk</i>	13.38	2.324
H229hjjk230	4	<i>hjjk</i>	16.38	2.173
H229hjkk231	4	<i>hjkk</i>	16.05	2.188
H229gkl232	3	<i>gkl</i>	14.30	2.274
H229dhjj233	4	<i>dhjj</i>	18.23	1.935
H229dffhjk234	7	<i>dffhjk</i>	20.38	2.097
H229fhikk235	5	<i>fhikk</i>	15.36	2.288
H229hkl236	3	<i>hkl</i>	16.40	2.172
H229fhjjk237	5	<i>fhjjk</i>	19.23	2.123
H229fghhjk238	6	<i>fghhjk</i>	20.89	2.065
H229fk239	3	<i>fkk</i>	11.26	2.150
H229ffhhij240	6	<i>ffhhij</i>	17.68	2.151
H229ffhhjk241	6	<i>ffhhjk</i>	18.72	2.110
H229ijk242	3	<i>ijk</i>	12.46	2.261
H229ffghj243	5	<i>ffghj</i>	19.07	1.886
H229hkk244	3	<i>hkk</i>	19.78	1.824
H229fghjk245	5	<i>fghjk</i>	14.68	2.217
H229ghkk246	4	<i>ghkk</i>	20.48	1.916
H229gkkk247	4	<i>gkkk</i>	17.62	2.121
H229hkkk248	4	<i>hkkk</i>	17.25	2.135
H229dfijk249	5	<i>dfijk</i>	17.23	2.153
H229ffhij250	5	<i>ffhij</i>	14.88	2.170
H229ghij251	4	<i>ghij</i>	14.43	2.153
H229ffhkk252	5	<i>ffhkk</i>	18.41	2.021
H229gjjj253	4	<i>gjjj</i>	16.57	2.164
H229gik254	3	<i>gik</i>	12.40	2.131
H229hkkk255	4	<i>hkkk</i>	16.54	2.166
H229ffgik256	5	<i>ffgik</i>	18.44	2.020
H229ffhhjk257	6	<i>ffhhjk</i>	16.69	2.193
H229jkk258	3	<i>jkk</i>	17.23	2.029

hypothetical structure	number of unique T atoms	WP combinations	Framework density /T nm ⁻³	<i>a</i> / nm
H229fhijk259	5	<i>fhijk</i>	19.89	2.099
H229gikk260	4	<i>gikk</i>	16.67	2.160
H229gij261	3	<i>gij</i>	14.22	2.036
H229ffhjk262	5	<i>ffhjk</i>	17.33	2.062
H229ghjk263	4	<i>ghjk</i>	15.27	2.113
H229hhjk264	4	<i>hhjk</i>	15.58	2.098
H229fjjk265	4	<i>fjjk</i>	18.70	2.045
H229ffjkk266	5	<i>ffjkk</i>	21.54	2.014
H229hjjk267	4	<i>hjjk</i>	20.27	2.024
H229fkl268	3	<i>fkl</i>	18.98	2.035
H229dijj269	4	<i>dijj</i>	17.39	2.078
H229ffghik270	6	<i>ffghik</i>	16.59	2.197
H229fhjk271	4	<i>fhjk</i>	17.40	1.985
H229djl272	3	<i>djl</i>	15.02	2.182
H229hjkk273	4	<i>hjkk</i>	15.15	2.230
H229l274	1	<i>l</i>	11.39	2.035
H229dhijj275	5	<i>dhijj</i>	18.10	2.150
H229fhik276	4	<i>fhik</i>	16.66	2.013
H229ffghkk277	6	<i>ffghkk</i>	22.92	1.973
H229dfjjk278	5	<i>dfjjk</i>	21.98	1.985
H229jkk279	3	<i>jkk</i>	15.06	2.122
H229dhjjj280	5	<i>dhjjj</i>	13.41	2.377
H229dij281	3	<i>dij</i>	12.00	2.080
H229gjkk282	4	<i>gjkk</i>	17.18	2.139
H229dffhjj283	6	<i>dffhjj</i>	16.01	2.172
H229hjjj284	4	<i>hjjj</i>	17.40	2.130
H229fgikk285	5	<i>fgikk</i>	19.46	2.114
H229fghjk286	5	<i>fghjk</i>	16.05	2.152
H229ffghjk287	6	<i>ffghjk</i>	17.77	2.147
H229fhijk288	5	<i>fhijk</i>	15.86	2.264
H229fgjk289	4	<i>fgjk</i>	16.29	2.029
H229fghhjk290	6	<i>fghhjk</i>	13.48	2.390
H229dhjjk291	5	<i>dhjjk</i>	16.73	2.207
H229djij292	4	<i>dijj</i>	14.54	2.205
H229dhijk293	5	<i>dhijk</i>	19.01	2.116
H229hijk294	4	<i>hijk</i>	18.59	2.083
H229hhjk295	4	<i>hhjk</i>	16.58	2.056
H229fhhjk296	5	<i>fhhjk</i>	15.47	2.179
H229jkk297	3	<i>jkk</i>	17.53	2.018
H229dhijk298	5	<i>dhijk</i>	19.81	2.087
H229ffkkk299	5	<i>ffkkk</i>	12.92	2.388
H229fjkk300	4	<i>fjkk</i>	17.42	2.094
H229ffhhjk301	6	<i>ffhhjk</i>	15.54	2.246
H229ffikk302	5	<i>ffikk</i>	19.44	2.084
H229hkkk303	4	<i>hkkk</i>	18.63	2.082
H229gijj304	4	<i>gijj</i>	17.49	2.126
H229fgijk305	5	<i>fgijk</i>	15.71	2.271
H229hjjj306	4	<i>hjjj</i>	17.93	2.108
H229gijk307	4	<i>gijk</i>	14.53	2.261
H229dhjkk308	5	<i>dhjkk</i>	18.55	2.133
H229gil309	3	<i>gil</i>	19.36	2.055
H229hkl310	3	<i>hkl</i>	14.29	2.274
H229ffkk311	4	<i>ffkk</i>	11.60	2.227
H229fhijk312	5	<i>fhijk</i>	12.42	2.456
H229ffjjk313	5	<i>ffjjk</i>	19.47	2.083
H229dhjkk314	5	<i>dhjkk</i>	17.44	2.177
H229gkkk315	4	<i>gkkk</i>	16.60	2.163
H229dffhhjj316	7	<i>dffhhjj</i>	15.94	2.277
H229fgik317	4	<i>fgik</i>	16.17	2.034
H229fhikk318	5	<i>fhikk</i>	16.41	2.238
H229ghi319	3	<i>ghi</i>	13.19	1.938
H229l320(KFI)	1	<i>l</i>	14.15	1.893