

Supplementary Information

A zeolite family with expanding structural complexity and embedded isoreticular structures

Peng Guo^{1,#}, Jiho Shin^{2,#}, Alex G. Greenaway³, Jung Gi Min², Jie Su¹, Hyun June Choi², Leifeng Liu¹, Paul A. Cox⁴, Suk Bong Hong^{2,*}, Paul A. Wright^{3,*}, Xiaodong Zou^{1,*}

¹ Inorganic and Structural Chemistry and Berzelii Centre EXSELENT on Porous Materials, Department of Materials and Environmental Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden.

² Centre for Ordered Nanoporous Materials Synthesis, School of Environmental Science and Engineering, POSTECH, Pohang 790-784, Korea.

³ EaStCHEM School of Chemistry, University of St. Andrews, St. Andrews, KY16 9ST, UK.

⁴ School of Pharmacy and Biomedical Sciences, University of Portsmouth, Portsmouth, PO1 2DT, UK.

These authors contributed equally to this work.

* Correspondence and requests for materials should be addressed to S.B.H. (sbhong@postech.ac.kr), P.A.W (paw2@st-andrews.ac.uk) or X.D.Z. (xzou@mmk.su.se).

Table of Contents

Section S1 Location of TEA ⁺ cations in NaTEA-ZSM-25 by computational modelling	S2-3
Figure S1-9	S3-11
Table S1-17	S12-54
References	S54

Section S1 Location of TEA⁺ cations in NaTEA-ZSM-25 by computational modelling

Taking the structural model of ZSM-25 derived from the RED data as a starting point, and including all elemental, solid state NMR and TGA analyses, the unit cell composition of the as-made NaTEA-ZSM-25 was deduced to be approximately $[(\text{N}(\text{C}_2\text{H}_5)_4)_{40}][\text{Na}_{285}\text{Al}_{325}\text{Si}_{1115}\text{O}_{2880}] \cdot (\text{H}_2\text{O})_{600}$. There are ca 40 TEA⁺ cations in the unit cell, which are present as extra-framework species along with Na⁺ cations and water molecules.

Due to the large number of guest molecules/cations in the structure, it is necessary to establish a good starting model of NaTEA-ZSM-25 prior to the Rietveld refinement. We first modelled the location of TEA⁺ cations using computational methods known from many previous studies to be a reliable method⁴²⁻⁴⁴. In this approach, the TEA⁺ cation positions were energy minimised via a molecular mechanics method based on the modified CVFF forcefield implemented in the program Materials Studio⁴⁵. A single TEA⁺ cation was docked into the appropriate cage within the unit cell. This ‘simulation box’ was then repeated to form an infinite array. Electrostatic and van der Waals energies were summed to infinity using the Ewald summation method. To ensure that charge of the simulation box was equal to zero, the charges of the anions were adjusted so that a compensating charge of -1.0 e was shared equally across all the framework oxygen ions. Prior to energy minimisation, each template was subject to a simulated annealing protocol that involved heating for 100,000 timesteps of duration 1×10^{-15} s at temperatures of 750, 500, 300 and 100 K. Conformations from this run were saved every 10,000 timesteps and each of these conformations was used as the starting point for an energy minimisation calculation. This procedure was repeated using several different starting positions within the appropriate cage.

The most favorable sites found by this approach are the *pau*, *t-plg* and *lta* cages in the structure, each of which is large enough that the TEA⁺ cation can be included without unfavorably close contacts. The modelled positions are shown in Figure S1, and the interaction energies are tabulated in Table S5. For the cages showing very favorable energies, the interaction is significantly more favorable with the slightly smaller *pau* and *t-plg* cages than with the larger *lta* cage. The interaction energies with the smaller *t-phi* and *t-gsm* cages are much less favorable, i.e., more positive (Table S5) because they are smaller and so unfavorable close contacts arise with TEA⁺.

We concluded from the modelling that the TEA⁺ cations could adopt sites in the *t-plg*, *pau* and *lta* cages. Since there are two *lta*, 18 *pau* and 24 *t-plg* cages and ca. 40 TEA⁺ cations per unit cell, it is likely that most of the *pau* and *t-plg* cages are occupied by TEA⁺ cations. Literature reports of zeolite syntheses in the presence of TEA⁺ support its likely templating role for *pau* cages. Merlinite (which contains *pau* cages) has been crystallised containing TEA⁺, and modelling studies suggested *pau* cages as its location⁴⁶. Synthetic paulingite, ECR-18, crystallises with included TEA⁺, and studies^{26,47} have shown that the number of TEA⁺ cations (24-26 per unit cell) requires the template to occupy both *pau* and *t-plg* cages (of which there are 12 and 16, respectively in each PAU unit cell), although additional occupancy of the *lta* cages cannot be ruled out. Furthermore, the silicoaluminophosphate STA-14, which has the KFI framework topology and so contains *pau* cages, is co-templated by TEA⁺. The

position and configuration of the template in the *pau* cages in STA-14 have been predicted by modelling and confirmed by single crystal X-ray diffraction to be the same as that modelled for TEA⁺ in the ZSM-25 structure⁴⁸.

Having established that it is likely that TEA⁺ cations occupy the *pau* and *t-plg* cages, we included them in these cages in our starting structural model for ZSM-25, with one TEA⁺ cation in each of the *pau* and *t-plg* cages. In addition, we added Na⁺ cations and guest water molecules according to previous refinements of the structurally similar paulingite⁴⁹, in other 8-ring sites throughout the structure and in the middle of the 6-ring positions in the *lta* cage.

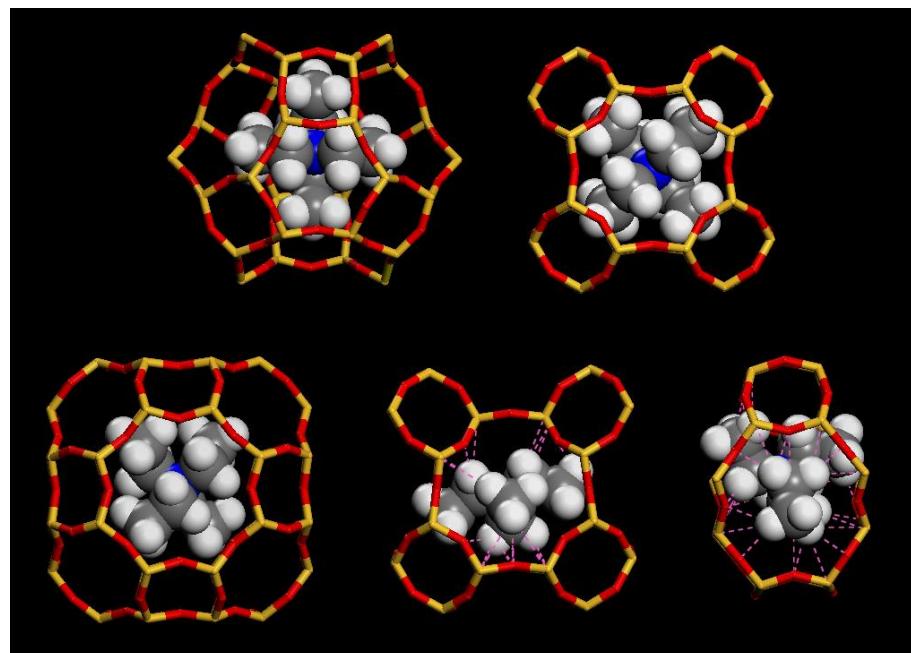


Figure S1 | Energy-minimised location of TEA⁺ cations in (clockwise, from top left) [4⁶6²8⁶] (*t-plg*), [4¹²8⁶] (*pau*), [4⁶8⁴] (*t-gsm*), [4⁷8⁵] (*t-phi*) and [4¹²6⁸8⁶] (*lta*) cages in the ZSM-25 framework. Dashed lines indicate energetically unfavorable close contacts.

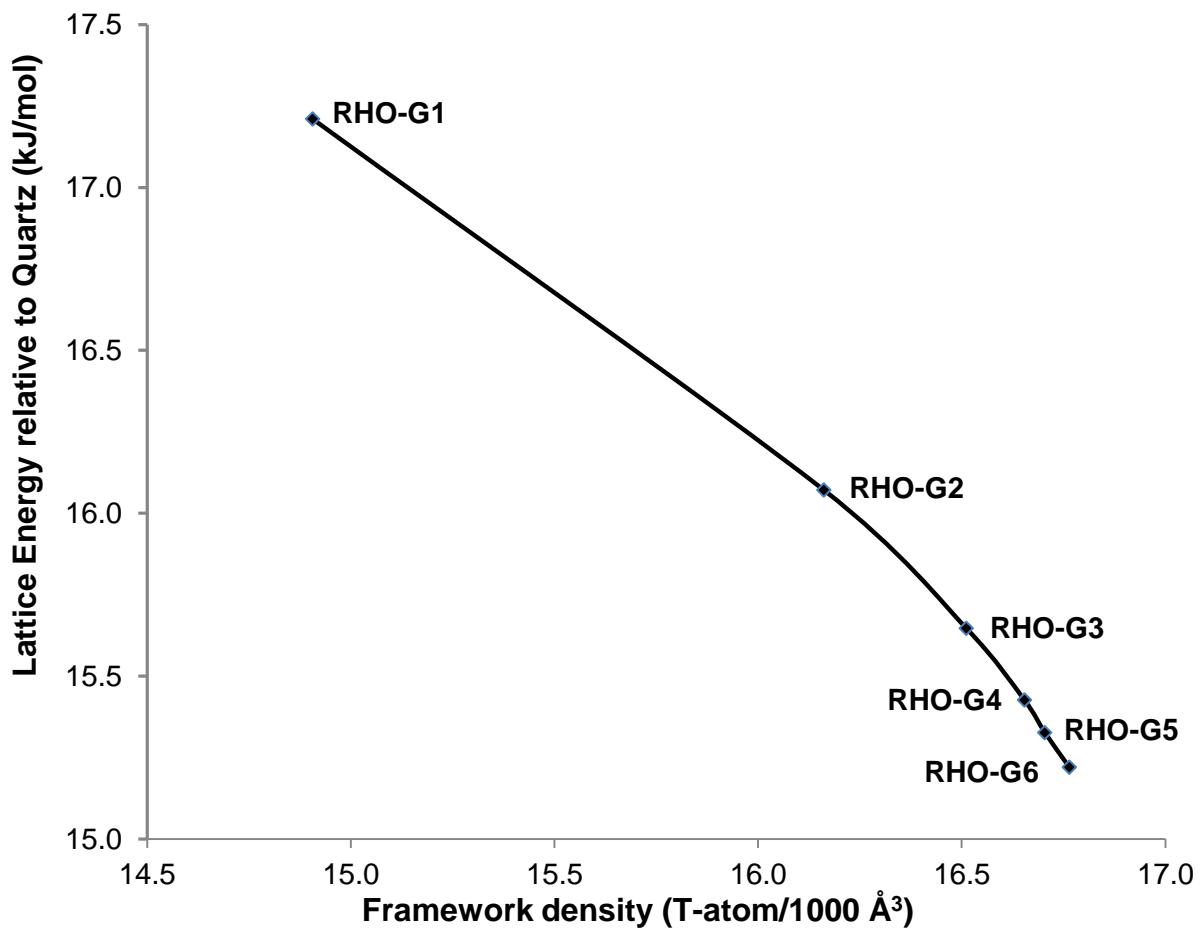


Figure S2 | Calculated lattice energy of the RHO-family relative to quartz as a function of framework density.

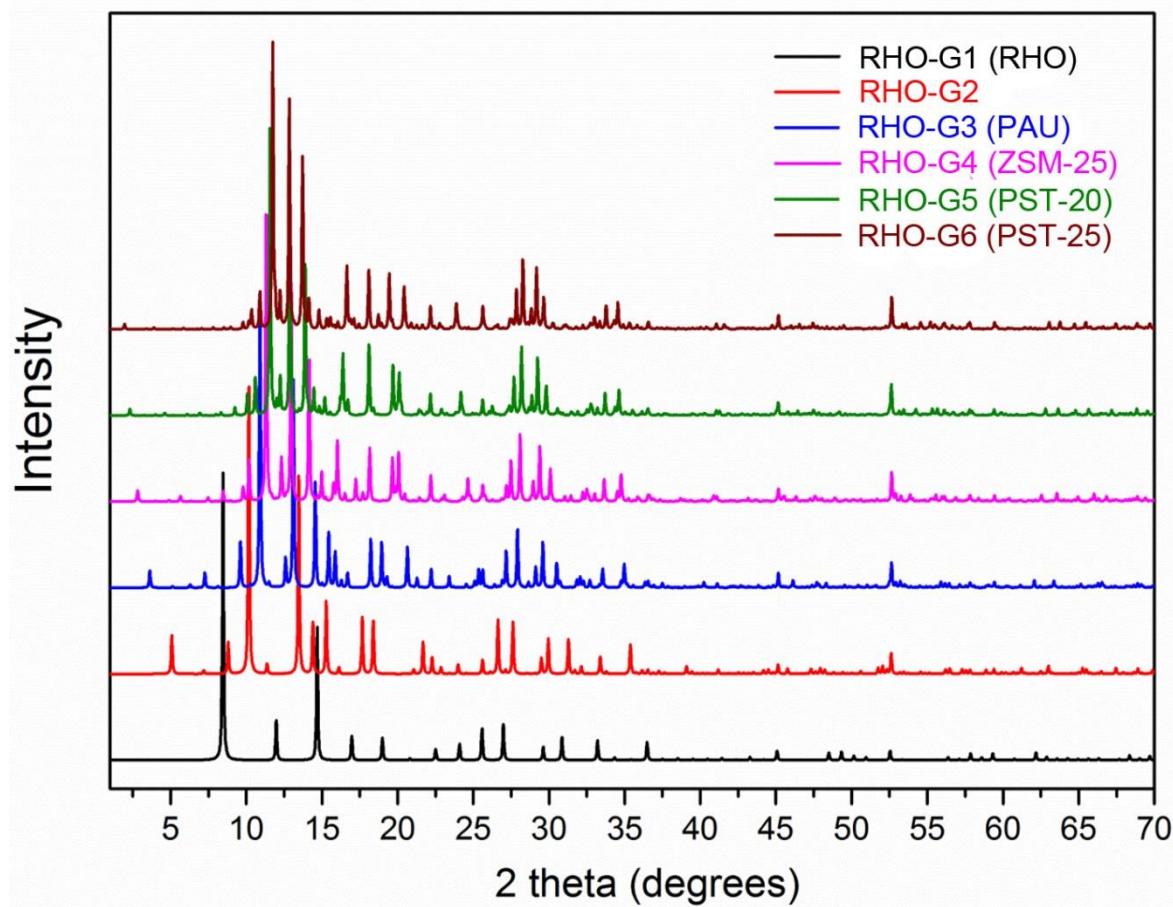


Figure S3 | Simulated powder X-ray diffraction patterns of RHO-family members RHO-G1-G6 ($\lambda = 1.54056 \text{ \AA}$).

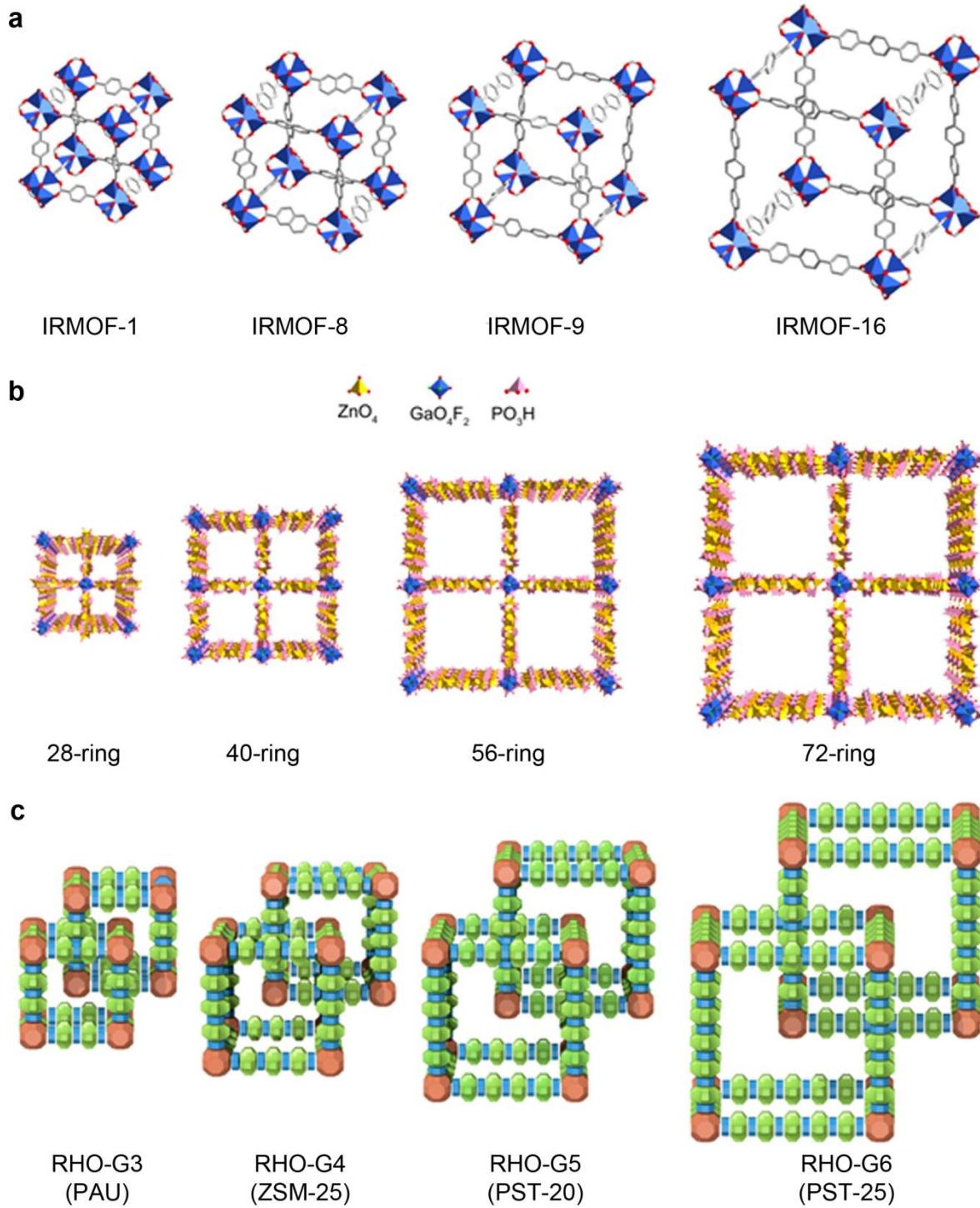


Figure S4 | Different principles of structure expansion. **a**, A family of isoreticular MOFs (IRMOF-*n*) by extending the length of the organic linker. IRMOF-9 has a double interpenetrated framework, and only one framework is shown for clarity^{2,3}. **b**, The gallium zincophosphite NTHU-13 family [A(BC)_nBA] with pore openings of 28, 40, 56, and 72-rings by inserting the chain building unit (BC)¹¹. **c**, The interpenetrated cubic scaffolds in zeolite RHO-family by inserting the *pau-d8r* unit on each unit cell edge and embedding the space by the *t-plg*, *t-oto*, *t-gsm*, and *t-phi* cages. The embedded cages are omitted for clarity.

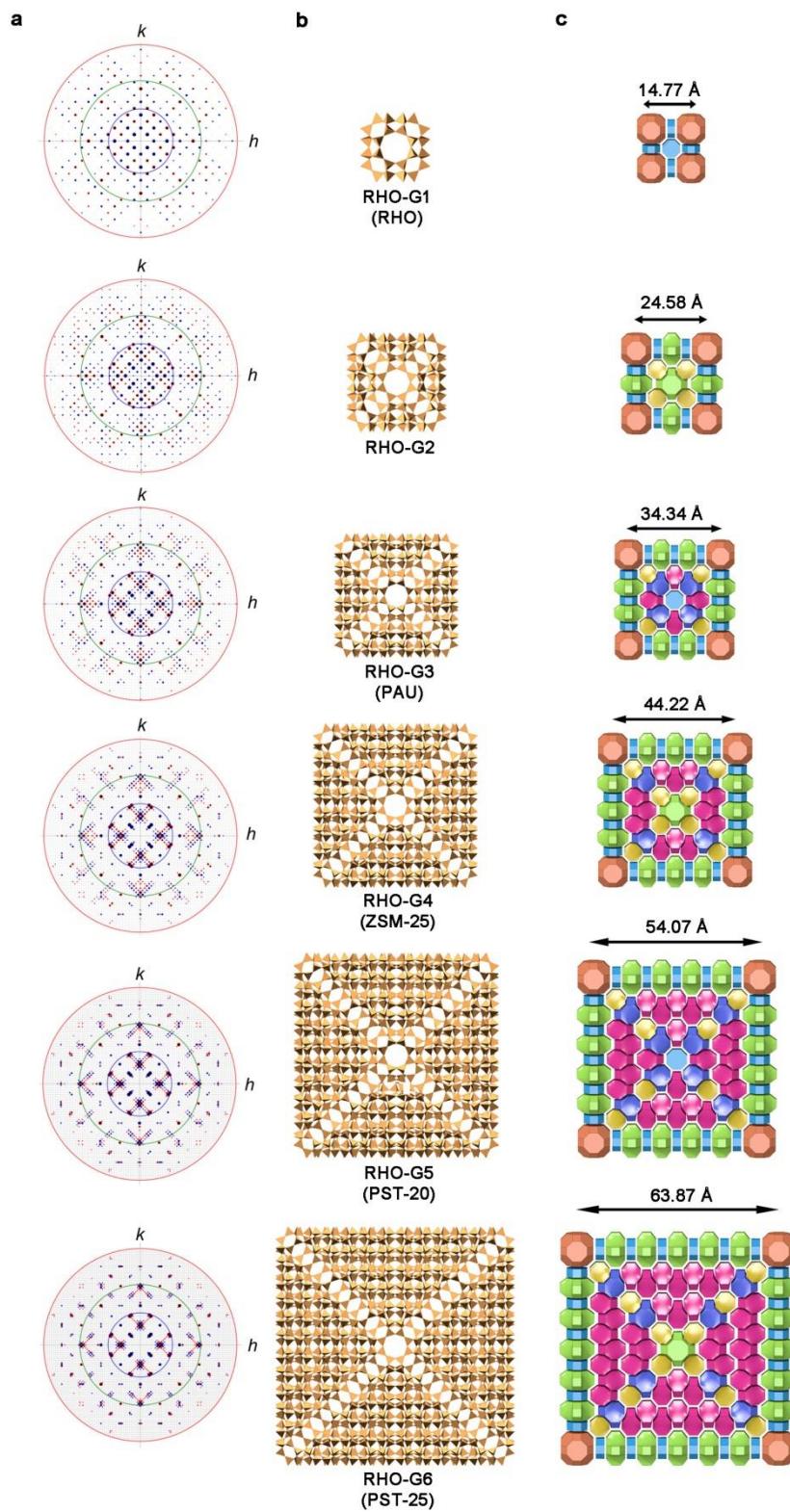


Figure S5 | Comparison of the reflection distributions and framework structures of the RHO family. **a**, The $(hk0)$ reciprocal plane showing that the distribution of strong reflections and the corresponding phases are similar for the four structures. Reflections in red have phases 0° , while those in blue have phases 180° . The red, green, and blue circles correspond to 1.0, 1.6 and 3.0 Å d-spacing. **b**, **c**, Polyhedral (**b**) and tiling (**c**) representation of cross-sections (about 12 Å thick) perpendicular to the c-axis of final structures.

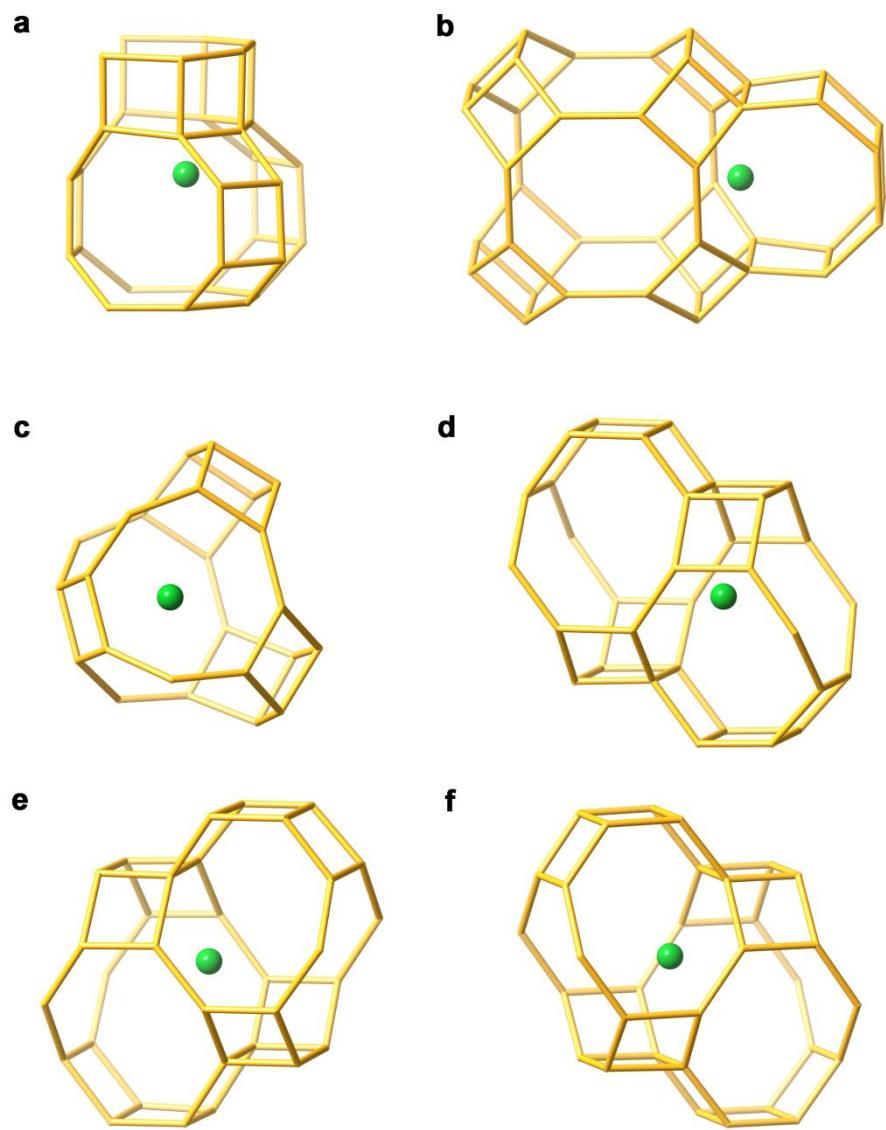


Figure S6 | Refined positions of Sr^{2+} cations within the as-made NaSrTEA-PST-20.
a, Cation site Sr1 in the 8-ring between a *t-oto* cage and a *t-phi* cage (48*k*, occupancy 0.46).
b, Cation site Sr2 in the 8-ring between a *t-phi* cage and a *pau* cage (48*k*, occupancy 0.46).
c, Cation site Sr3 in a *t-phi* cage (48*k*, occupancy 0.85). **d**, Cation site Sr4 in the 8-ring between two *t-gsm* cages (48*j*, occupancy 0.60). **e**, Cation site Sr5 in the 8-ring between two *t-gsm* cages (96*l*, occupancy 0.60). **f**, Cation site Sr6 in the 8-ring between two *t-gsm* cages (48*j*, occupancy 1.00).

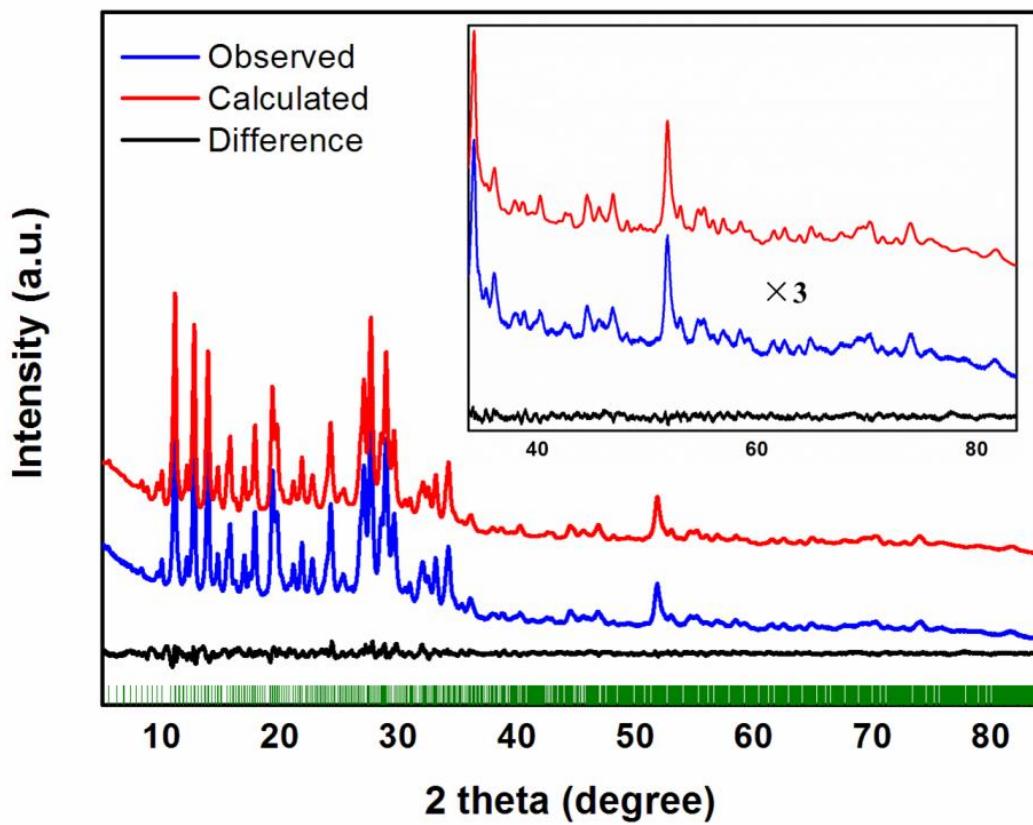


Figure S7 | Rietveld refinement of calcined, hydrated ZSM-25. The observed, calculated and difference curves are in blue, red and black, respectively. The green vertical bars indicate the positions of Bragg peaks ($\lambda = 1.5418 \text{ \AA}$).

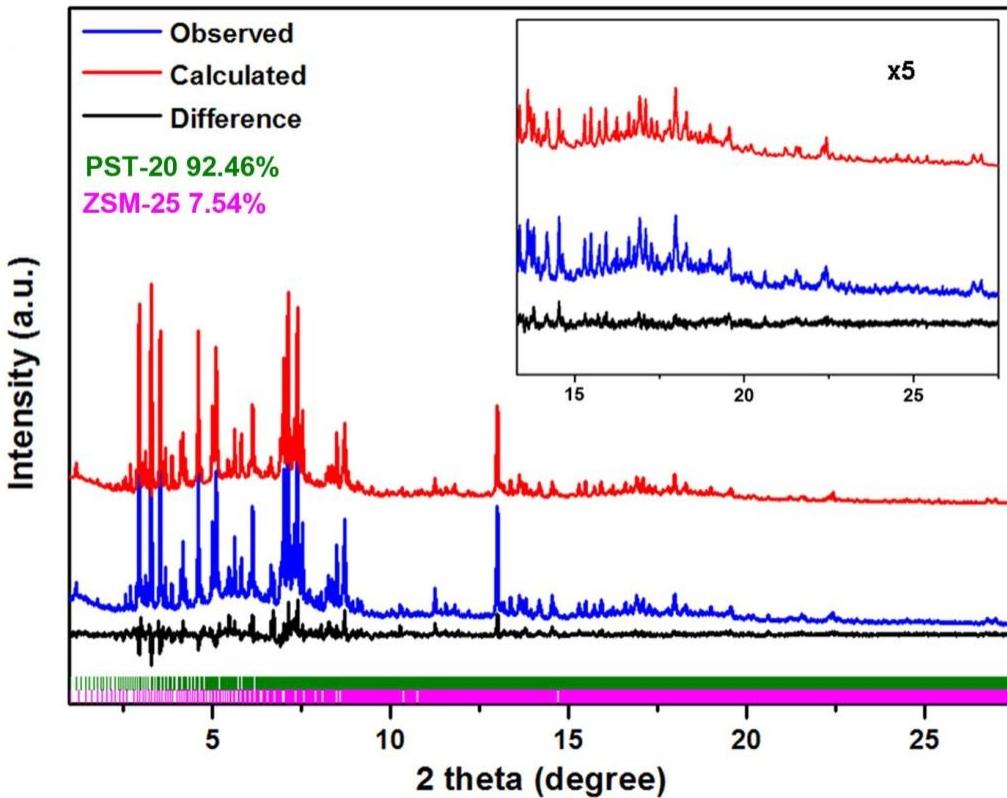


Figure S8 | Rietveld refinement of Na^+ -exchanged NaSrTEA-PST-20 based on two phases NaTEA-PST-20 and NaTEA-ZSM-25 . The observed, calculated and difference curves are in blue, red and black, respectively. The green vertical bars indicate the positions of Bragg peaks ($\lambda = 0.40091 \text{ \AA}$).

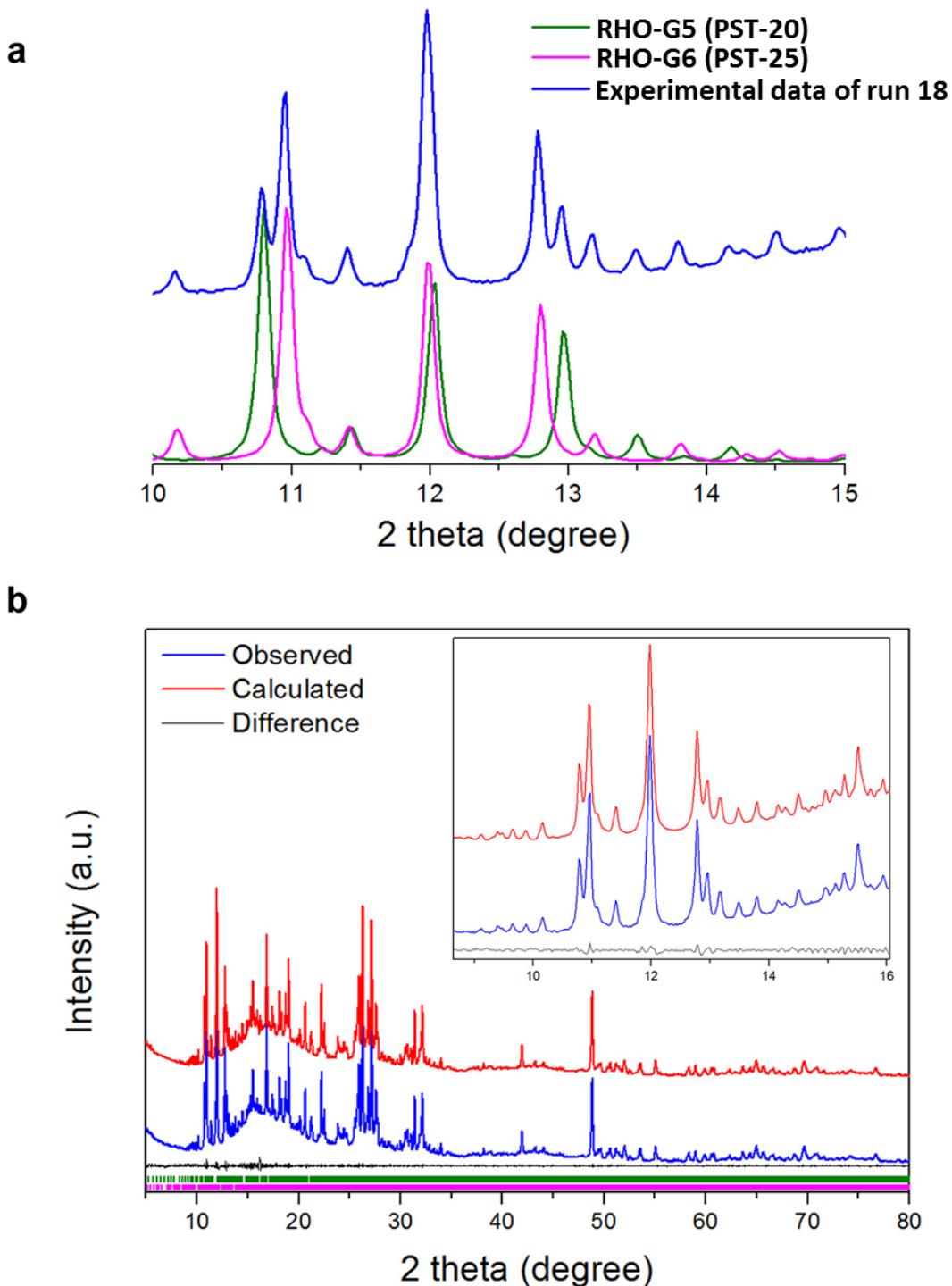


Figure S9 | a, Synchrotron PXRD pattern of the sample obtained from run 18 in Table S3. Simulated PXRD patterns of PST-20 and PST-25 are shown by green and pink lines, respectively ($\lambda = 1.4640 \text{ \AA}$). Based on the peak intensities, ca 75% of PST-25 and 25% of ZSM-25 are estimated in the sample. **b**, LeBail profile fit using two phases of PST-20 and PST-25. The refinement yielded the following unit cell parameters: PST-20 ($Im\text{-}3m$, $a = 55.0270(5) \text{ \AA}$) and PST-25 ($Im\text{-}3m$, $a = 65.0436(4) \text{ \AA}$). The observed, calculated and difference curves are in blue, red and black, respectively. Green and pink vertical bars indicate the positions of Bragg peaks of PST-20 and PST-25, respectively.

Table S1 | Representative Synthesis Results.*

Run	M _{II}	Product [†]
1	-	ZSM-25
2	Mg	Amorphous
3	Ca	Gismondine + PST-20 + ZSM-25
4	Sr	PST-20 + ZSM-25 + analcime
5 [‡]	Sr	Amorphous
6	Ba	Analcime + PST-20 + ZSM-25

*The oxide composition of synthesis mixture is 5.2TEABr•1.9Na₂O•0.5M_{II}(NO₃)₂•1.0Al₂O₃•7.2SiO₂•390H₂O, where M_{II} is Mg²⁺, Ca²⁺, Sr²⁺, or Ba²⁺. Crystallisation was performed under rotation (60 rpm) at 413 K for 7 days, unless otherwise stated.

[†]The phase appearing first is the major phase.

[‡]Run performed under static conditions.

Table S2 | Syntheses of PST-20 from gel composition of 5.2TEABr•1.9Na₂O•0.5Sr(NO₃)₂•1.0Al₂O₃•7.2SiO₂•390H₂O.

Run	Temp (K)	Time (days)	Product [*]
7	373	14	Amorphous
8	408	4	ZSM-25 + PST-20
9	413	4	PST-20 + ZSM-25
10	418	4	PST-20 + (ZSM-25)
11 [†]	418	2	PST-20
12 [†]	418	7	PST-20 + analcime
13	423	14	Amorphous
14	448	14	Amorphous

^{*}The phase appearing first is the major phase, and the product obtained in a trace amount is given in parentheses.

[†]Run performed after adding a small amount (2 wt% of anhydrous raw materials) of the material which was obtained from Run 4 as seeds to the synthesis mixture.

Table S3 | Syntheses from gel composition of 5.2TEABr•1.9Na₂O•xM_{II}(NO₃)₂•1.0Al₂O₃•7.2SiO₂•yH₂O.^{*}

Run	<i>x</i>		<i>y</i>	Product [†]
	M _{II} = Sr	M _{II} = Ca		
15	0.50	-	390	PST-20 + (ZSM-25)
16	0.50	-	300	PST-20 + (analcime)
17	0.50	-	250	Gismondine + U _I [‡]
18	0.25	0.25	250	PST-25 + PST-20
19	-	0.50	250	U _{II} [§] + PST-25 + (gismondine)
20	0.25	0.25	200	Gismondine

^{*}Crystallisation was performed under rotation (60 rpm) at 418 K for 2 days.

[†]The phase appearing first is the major phase.

[‡]Unknown, probably dense material.

[§]Unknown.

Table S4 | Experimental parameters for RED data collection and crystallographic data for as-made NaTEA-ZSM-25 and NaSrTEA-PST-20 ($\lambda = 0.0251$ Å).

Sample	NaTEA-ZSM-25	NaSrTEA-PST-20
Tilt range (°)	-42.02° to 34.69°	22.06° to -27.92°
Tilt step (°)	0.1	0.2
Exposure time/frame (s)	3	1
Total number of frames	798	275
Data collection time (min)	70	17
Crystal system	Cubic	
Possible space groups	<i>I</i> 432 (No. 211), <i>I</i> -43 <i>m</i> (No. 217), <i>Im</i> -3 <i>m</i> (No. 229)	
Unit cell parameter <i>a</i> obtained from RED (Å) ^a	42.3	52.4
Volume (Å ³)	75860.8	143877.8
Resolution (Å)	2.2	2.5
Completeness (%)	77.8	84.1

^aThe unit cell parameter obtained after Rietveld refinement against the synchrotron PXRD pattern was $a = 45.0711(3)$ Å for NaTEA-ZSM-25 (Supplementary Table 6) and $55.0430(17)$ Å for NaSrTEA-PST-20 (Supplementary Table 8). The reduction of the unit cell parameter in the TEM was likely due to the removal of water molecules in vacuum and by electron beam.

Table S5 | Calculated interaction energies of TEA⁺ cations in different cages in the ZSM-25 framework.

Cage type	Interaction energy of TEA ⁺ / kcal mol ⁻¹
[4 ⁶ 6 ² 8 ⁶] (<i>t-plg</i>)	-52.7
[4 ¹² 8 ⁶] (<i>pau</i>)	-51.8
[4 ¹² 6 ⁸ 8 ⁶] (<i>lta</i>)	-39.6
[4 ⁷ 8 ⁵] (<i>t-phi</i>)	-3.7
[4 ⁶ 8 ⁴] (<i>t-gsm</i>)	8.6

Table S6 | Crystallographic details for the refinement of as-made NaTEA-ZSM-25.

NaTEA-ZSM-25	
Measured chemical formula (sum)	$ (N(C_2H_5)_4)_{40}Na_{285}(H_2O)_{600} [Al_{325}Si_{1115}O_{2880}]$
Refined chemical formula (sum) [*]	$ (N(C_2H_5)_4)_{38}Na_{296}(H_2O)_{812} [Al_{334}Si_{1106}O_{2880}]$
Diffractometer	Synchrotron X-ray, ID-31, ESRF, Grenoble
Wavelength	0.632480 Å
Space Group	<i>Im-3m</i>
<i>a</i> / Å	45.0711(3)
Number of reflections	8080
Number of parameters	242
Number of restraints	202 (96 for O-T-O, 64 for T-O, 28 for TEA, 8 for Na-O, 4 for Na-Na and 2 for O-O)
R _p	0.0414
R _{wp}	0.0537
GOF	2.87

* Hydrogen atoms were not included in the refinement, but added afterwards.

Table S7 | Crystallographic details for the refinement of calcined ZSM-25^{*}.

Calcined ZSM-25	
Measured chemical formula (sum)	[Na ₂₈₅ (H ₂ O) ₈₈₀][H ₄₀ Al ₃₂₅ Si ₁₁₁₅ O ₂₈₈₀]
Refined chemical formula (sum) **	[Na ₂₈₅ (H ₂ O) ₈₄₆][H ₄₀ Al ₃₂₅ Si ₁₁₁₅ O ₂₈₈₀]
Diffractometer	PANalytical X’Pert PRO diffractometer
Wavelength	1.5418 Å
Space Group	<i>Im-3m</i>
<i>a</i> / Å	44.9242(16)
Number of reflections	3001
Number of parameters	233
Number of restraints	174 (96 for O-T-O, 64 for T-O, 8 for Na-O, 4 for Na-Na and 2 for O-O)
R _p	0.0265
R _{wp}	0.0340
GOF	3.86

* The as-made NaTEA-ZSM-25 was calcined in air at 773 K for 8 h with a ramping rate of 2 K min⁻¹. After calcination, the sample was exposed to the laboratory humidity conditions for 1 d. The PXRD pattern was obtained in flat plate mode in air.

** Hydrogen atoms were not included in the refinement, but added afterwards.

Table S8 | Crystallographic details for the refinement of as-made NaSrTEA-PST-20.

NaSrTEA-PST-20	
Measured chemical formula (sum)	$[(\text{N}(\text{C}_2\text{H}_5)_4)_{56}\text{Na}_{194}\text{Sr}_{194}(\text{H}_2\text{O})_{600}[\text{Al}_{638}\text{Si}_{2002}\text{O}_{5280}]]$
Refined chemical formula (sum) [*]	$[(\text{N}(\text{C}_2\text{H}_5)_4)_{56}\text{Na}_{162}\text{Sr}_{210}(\text{H}_2\text{O})_{563}[\text{Al}_{638}\text{Si}_{2002}\text{O}_{5280}]]$
Diffractometer	Synchrotron X-ray, ID-22, ESRF, Grenoble
Wavelength	0.40091 Å
Space Group	<i>Im-3m</i>
<i>a</i> / Å	55.0437(16)
Number of reflections	13872
Number of parameters	372
Number of restraints	298 (174 for O-T-O, 116 for T-O, 8 for Na/Sr – H ₂ O/TEA)
R _p	0.0569
R _{wp}	0.0791
GOF	4.396

* Hydrogen atoms were not included in the refinement, but added afterwards.

Table S9 | Crystallographic details for the refinements of Na⁺-exchanged NaSrTEA-PST-20 (denoted NaTEA-PST-20) with one or two phases.

	One phase (NaTEA-PST-20)	Two phases (NaTEA-PST-20 and NaTEA-ZSM-25)
Diffractometer	Synchrotron X-ray, ID-22, ESRF, Grenoble	Synchrotron X-ray, ID-22, ESRF, Grenoble
Wavelength	0.40091Å	0.40091Å
Space Group	<i>Im-3m</i>	<i>Im-3m</i> (for both PST-20 and ZSM-25)
<i>a</i> / Å	55.0664(7)	55.080(1) (PST-20) 45.063(4) (ZSM-25)
Number of reflections	13883	13895 (PST-20) 7744 (ZSM-25)
Number of parameters	333	51
Number of restraints	318 (174 for O-T-O, 116 for T-O, 28 for TEA)	The atomic position and thermal parameters are fixed based on the previous structure models.
R _p	0.06528	0.05932
R _{wp}	0.08828	0.07927
GOF	3.589	3.155

Table S10 | The coordination sequences and vertex symbols of the RHO-G4 (ZSM-25) framework. The framework density FD is 15.7 Si atoms/1000Å³, TD10 = 735.

T-atom	Coordination sequences	Vertex symbols
Si1	4 9 18 32 49 70 95 123 156 193	4.4.4.8 ₂ .8.8
Si2	4 9 18 32 49 69 94 123 154 189	4.4.4.8 ₂ .8.8
Si3	4 9 18 32 48 67 92 121 152 186	4.4.4.8 ₂ .8.8
Si4	4 9 18 31 47 68 92 119 152 188	4.4.4.8 ₂ .8.8
Si5	4 9 17 29 45 65 89 117 149 185	4.4.4.6.8.8
Si6	4 9 18 32 49 70 96 124 156 194	4.4.4.8 ₂ .8.8
Si7	4 9 18 32 49 70 96 125 157 193	4.4.4.8 ₂ .8.8
Si8	4 9 18 31 47 68 92 118 150 185	4.4.4.8 ₂ .8.8
Si9	4 9 18 31 47 68 91 116 149 187	4.4.4.8 ₂ .8.8
Si10	4 9 17 30 47 66 88 114 145 181	4.4.4.6.8.8
Si11	4 9 18 32 49 69 94 122 152 187	4.4.4.8 ₂ .8.8
Si12	4 9 18 32 48 67 91 120 157 196	4.4.4.8 ₂ .8.8
Si13	4 9 18 32 49 69 95 126 158 194	4.4.4.8 ₂ .8.8
Si14	4 9 18 32 49 68 93 123 152 188	4.4.4.8 ₂ .8.8
Si15	4 9 18 32 48 68 93 121 151 183	4.4.4.8 ₂ .8.8
Si16	4 9 18 32 48 69 96 123 157 194	4.4.4.8 ₂ .8.8

Point symbol for the net: (4³.6².8)₁₃(4³.6³)₂

Transitivity 16 40 39 15

Table S11 | The coordination sequences and vertex symbols of the RHO-G5 (PST-20) framework. The framework density FD is 15.8 Si atoms/1000Å³, TD10 =737.

T-atom	Coordination sequences	Vertex symbols
Si1	4 9 18 32 49 70 96 125 158 196	4.4.4.8 ₂ .8.8
Si2	4 9 18 32 48 67 92 120 154 194	4.4.4.8 ₂ .8.8
Si3	4 9 18 31 47 68 92 117 148 184	4.4.4.8 ₂ .8.8
Si4	4 9 18 32 49 70 96 125 158 195	4.4.4.8 ₂ .8.8
Si5	4 9 18 32 48 67 94 128 162 195	4.4.4.8 ₂ .8.8
Si6	4 9 18 32 49 69 93 121 152 186	4.4.4.8 ₂ .8.8
Si7	4 9 17 30 47 66 88 115 146 179	4.4.4.6.8.8
Si8	4 9 18 32 49 69 94 125 158 193	4.4.4.8 ₂ .8.8
Si9	4 9 18 32 49 70 95 123 156 193	4.4.4.8 ₂ .8.8
Si10	4 9 18 32 49 69 94 123 154 189	4.4.4.8 ₂ .8.8
Si11	4 9 18 32 48 67 92 121 152 186	4.4.4.8 ₂ .8.8
Si12	4 9 18 31 47 68 92 119 152 188	4.4.4.8 ₂ .8.8
Si13	4 9 17 29 45 65 89 117 149 185	4.4.4.6.8.8
Si14	4 9 18 31 47 68 92 118 150 185	4.4.4.8 ₂ .8.8
Si15	4 9 18 31 47 68 91 116 149 187	4.4.4.8 ₂ .8.8
Si16	4 9 17 30 47 66 88 114 145 181	4.4.4.6.8.8
Si17	4 9 18 32 49 69 94 122 152 187	4.4.4.8 ₂ .8.8
Si18	4 9 18 32 48 67 91 121 157 193	4.4.4.8 ₂ .8.8
Si19	4 9 18 32 49 70 96 124 156 194	4.4.4.8 ₂ .8.8
Si20	4 9 18 32 49 70 96 125 157 194	4.4.4.8 ₂ .8.8
Si21	4 9 18 32 49 69 95 125 157 194	4.4.4.8 ₂ .8.8
Si22	4 9 18 32 48 69 96 123 155 192	4.4.4.8 ₂ .8.8
Si23	4 9 18 32 48 68 93 121 151 184	4.4.4.8 ₂ .8.8
Si24	4 9 18 32 49 68 93 123 153 188	4.4.4.8 ₂ .8.8
Si25	4 9 18 32 48 68 95 123 156 198	4.4.4.8 ₂ .8.8
Si26	4 9 18 32 49 69 93 121 152 190	4.4.4.8 ₂ .8.8
Si27	4 9 18 32 48 67 91 119 153 190	4.4.4.8 ₂ .8.8
Si28	4 9 18 32 49 69 94 123 154 189	4.4.4.8 ₂ .8.8
Si29	4 9 18 32 49 68 93 123 152 186	4.4.4.8 ₂ .8.8

Point symbol for the net: (4³.6².8)₁₀(4³.6³)

Transitivity 29 70 65 22

Table S12 | Energy minimisation of the RHO-Gn structures in the RHO-family by GULP.

Zeolite	a (Å)*	V (Å ³)*	Number of Si atoms per unit cell	Framework density (T atom/1000 Å ³)	Lattice Energy relative to Quartz (kJ/mol)
RHO-G1 (RHO)	14.77	3220.22	48	14.91	17.21
RHO-G2	24.58	14851.02	240	16.16	16.07
RHO-G3 (PAU)	34.40	40699.42	672	16.51	15.65
RHO-G4 (ZSM-25)	44.22	86466.40	1440	16.65	15.43
RHO-G5 (PST-20)	54.07	158049.10	2640	16.70	15.33
RHO-G6 (PST-25)	63.87	260554.70	4368	16.76	15.22
Quartz			3	27.67	0

*Via constant pressure GULP energy minimisation.

Table S13 | Occurrence of different cages per unit cell in the RHO-Gn structure of the RHO-family.*

	n	 [4 ¹² 6 ⁸ 8 ⁶] <i>lta</i>	 [4 ⁸ 8 ²] <i>d8r</i>	 [4 ¹² 8 ⁶] <i>pau</i>	 [4 ⁶ 6 ² 8 ⁶] <i>t-plg</i>	 [4 ⁵ 8 ³] <i>t-oto</i>	 [4 ⁶ 8 ⁴] <i>t-gsm</i>	 [4 ⁷ 8 ⁵] <i>t-phi</i>
RHO-G1 (RHO)	0	2	6	0	0	0	0	0
RHO-G2	1	2	12	6	8	24	0	0
RHO-G3 (PAU)	2	2	18	12	16	72	12	24
RHO-G4 (ZSM-25)	3	2	24	18	24	144	60	72
RHO-G5 (PST-20)	4	2	30	24	32	240	168	144
RHO-G6 (PST-25)	5	2	36	30	40	360	360	240

*The number of cages was calculated according to the following: $N_{d8r} = 6n$; $N_{pau} = 6(n-1)$; $N_{t-plg} = 8(n-1)$; $N_{t-oto} = 12n(n-1)$; $N_{t-gsm} = 2(n-1)(n-2)(2n-3)$; $N_{t-phi} = 12(n-1)(n-2)$. The number of *lta* cages is two for all the members in the RHO-family.

Table S14. The number of cages (tiles) in the asymmetric unit of the RHO-Gn structure in the RHO-family.

	 [4 ¹² 6 ⁸ 8 ⁶] <i>lta</i>	 [4 ⁸ 8 ²] <i>d8r</i>	 [4 ¹² 8 ⁶] <i>pau</i>	 [4 ⁶ 6 ² 8 ⁶] <i>t-plg</i>	 [4 ⁵ 8 ³] <i>t-oto</i>	 [4 ⁶ 8 ⁴] <i>t-gsm</i>	 [4 ⁷ 8 ⁵] <i>t-phi</i>
RHO-G1	1	1	0	0	0	0	0
RHO-G2	1	1	1	1	1	0	0
RHO-G3	1	2	1	1	2	1	1
RHO-G4	1	2	2	2	4	2	2
RHO-G5	1	3	2	2	6	4	4
RHO-G6	1	3	3	3	9	7	6

Table S15. Prediction of structure factor amplitudes and phases of strong reflections in RHO-G4 (ZSM-25) from those calculated from the RHO-G3 structure. This is done by converting the reflection indices of RHO-G3 to RHO-G4 according to the relationship: $h_{\text{RHO-G4}} = h_{\text{RHO-G3}} \times a_{\text{RHO-G4}} / a_{\text{RHO-G3}}$, $k_{\text{RHO-G4}} = k_{\text{RHO-G3}} \times a_{\text{RHO-G4}} / a_{\text{RHO-G3}}$, $l_{\text{RHO-G4}} = l_{\text{RHO-G3}} \times a_{\text{RHO-G4}} / a$ ($a_{\text{RHO-G3}} = 35 \text{ \AA}$ and $a_{\text{RHO-G4}} = 45 \text{ \AA}$), and then transposing the corresponding structure factor amplitudes and phases of RHO-G3 to RHO-G4. 133 reflections with normalised structure factor $E > 1.2$ and $d > 1.00 \text{ \AA}$ were selected.

$h_{\text{RHO-G3}}$	$k_{\text{RHO-G3}}$	$l_{\text{RHO-G3}}$	E-value	$h_{\text{RHO-G4}}$	$k_{\text{RHO-G4}}$	$l_{\text{RHO-G4}}$	Amplitude	Phase	$d_{\text{RHO-G3}} (\text{\AA})$
3	3	0	1.38	4	4	0	979	180	8.25
4	3	1	1.42	5	4	1	502	0	6.86
10	3	1	1.75	13	4	1	409	180	3.34
10	4	0	2.25	13	5	0	746	0	3.25
11	3	0	2.04	14	4	0	674	0	3.07
11	4	1	1.50	14	5	1	350	180	2.98
11	6	3	1.48	14	8	4	345	180	2.72
10	8	4	2.44	13	10	5	389	180	2.61
14	0	0	1.47	18	0	0	662	180	2.50
10	10	6	1.85	13	13	8	268	180	2.28
14	7	1	2.01	18	9	1	205	0	2.23
14	7	7	2.37	18	9	9	461	180	2.04
17	2	1	1.33	22	3	1	183	180	2.04
13	11	4	1.31	17	14	5	180	0	2.00
13	12	3	1.24	17	15	4	170	180	1.95
14	11	3	1.41	18	14	4	193	180	1.94
17	6	3	1.31	22	8	4	180	0	1.92
18	5	1	1.23	23	6	1	108	180	1.87
17	7	4	1.39	22	9	5	121	180	1.86
19	1	0	1.59	25	1	0	196	0	1.84
19	3	0	1.47	24	4	0	182	180	1.82
14	14	0	2.04	18	18	0	894	0	1.77
20	0	0	1.24	26	0	0	766	0	1.75
14	11	11	2.08	18	14	14	348	0	1.67
21	1	0	1.90	27	1	0	317	180	1.66
15	11	10	1.27	19	14	13	150	180	1.66
14	14	8	1.35	18	18	10	227	180	1.64
21	4	3	1.90	27	5	4	225	0	1.62
22	0	0	1.32	28	0	0	462	0	1.59
21	7	0	2.40	27	9	0	420	0	1.58
22	4	4	1.34	28	5	5	180	180	1.54
20	11	3	2.45	26	14	4	232	0	1.52
18	14	4	1.68	23	18	5	160	180	1.51
21	10	3	3.11	27	13	4	295	180	1.49
22	9	3	1.49	28	12	4	141	180	1.46
21	11	4	1.84	27	14	5	174	180	1.46
24	3	1	1.21	31	4	1	114	0	1.45

14	14	14	1.23	18	18	18	285	180	1.44
24	4	0	1.67	31	5	0	223	180	1.44
20	14	0	2.04	26	18	0	280	180	1.43
22	10	4	2.29	28	13	5	222	0	1.43
17	13	12	1.29	22	17	15	125	180	1.43
23	8	3	1.34	30	10	4	129	180	1.43
17	17	6	1.44	22	22	8	198	0	1.41
21	14	1	2.14	27	18	1	213	0	1.39
20	11	11	1.23	26	14	14	173	180	1.38
24	8	4	1.84	31	10	5	183	0	1.37
18	17	7	2.26	23	22	9	225	180	1.36
21	11	10	2.01	27	14	13	200	0	1.36
25	6	3	1.26	32	8	4	145	0	1.35
24	10	0	1.82	31	13	0	296	0	1.35
22	14	0	1.81	28	18	0	293	180	1.34
22	10	10	2.11	28	13	13	342	180	1.34
24	11	1	1.24	31	14	1	143	180	1.32
23	10	9	2.29	29	13	12	186	180	1.31
18	18	8	1.49	23	23	10	171	0	1.31
24	10	6	1.23	31	13	8	100	0	1.31
19	17	8	1.23	24	22	10	100	180	1.31
23	11	8	1.29	30	14	10	105	0	1.31
25	10	1	1.40	32	13	1	114	180	1.30
21	17	2	1.35	27	22	3	110	180	1.29
24	9	9	1.58	30	12	12	182	180	1.29
24	10	8	3.12	31	13	10	342	180	1.29
25	11	0	1.59	32	14	0	247	0	1.28
24	11	7	1.70	31	14	9	187	0	1.28
25	10	7	2.02	32	13	9	222	0	1.26
25	11	6	2.26	32	14	8	246	180	1.25
28	0	0	1.22	36	0	0	375	0	1.25
20	14	14	1.50	26	18	18	231	0	1.24
21	14	13	1.55	27	18	17	169	180	1.23
21	16	11	1.62	27	21	14	147	180	1.22
25	14	3	1.85	32	18	4	168	0	1.21
28	7	1	3.27	36	9	1	296	0	1.21
21	18	9	1.73	27	23	12	161	0	1.20
28	8	0	2.08	36	10	0	274	180	1.20
22	17	9	1.22	28	22	12	114	180	1.20
24	13	11	1.38	31	17	14	128	0	1.19
27	11	4	1.30	35	14	5	121	180	1.19
21	17	12	1.62	27	22	15	150	0	1.18
20	19	11	1.72	26	24	14	196	0	1.18
28	7	7	2.64	36	9	9	425	180	1.18
21	20	7	1.59	27	26	9	180	0	1.17
21	19	10	1.58	27	24	13	179	180	1.17

21	21	6	2.05	27	27	8	150	180	1.16
21	20	9	2.31	27	11	12	120	180	1.15
23	20	1	1.20	30	25	1	62	0	1.15
25	16	7	1.40	32	21	9	73	180	1.15
21	21	8	3.02	27	27	10	402	180	1.14
22	19	11	1.44	28	24	14	136	0	1.13
27	14	7	1.81	35	18	9	128	180	1.12
28	14	0	2.39	36	18	0	241	180	1.12
24	20	2	1.34	31	26	3	96	0	1.12
20	20	14	1.43	26	26	18	144	180	1.11
22	21	9	1.43	28	27	11	91	180	1.10
21	20	13	1.30	27	26	17	83	0	1.10
26	17	7	1.20	33	22	9	77	0	1.10
30	11	1	1.79	39	14	1	114	0	1.09
21	21	12	1.80	27	27	14	161	180	1.09
24	21	3	1.84	31	27	4	117	0	1.09
22	20	12	1.50	28	26	14	95	0	1.09
25	20	3	1.94	32	26	4	113	180	1.09
26	18	6	1.42	33	23	8	83	180	1.09
20	18	18	1.33	26	23	23	109	0	1.08
23	20	11	1.77	30	26	14	103	0	1.08
21	18	17	2.05	27	23	22	120	180	1.08
28	15	7	1.97	36	19	9	115	0	1.08
24	22	4	1.89	31	28	5	151	180	1.07
21	21	14	1.97	27	27	18	224	0	1.07
22	20	14	1.42	28	26	18	114	180	1.07
25	21	4	2.21	32	27	5	177	0	1.06
31	11	0	1.57	40	14	0	177	0	1.06
24	18	14	1.38	31	23	18	66	180	1.06
24	21	9	1.47	31	27	12	70	0	1.06
32	8	4	1.22	41	10	5	58	180	1.05
24	19	13	1.40	31	24	17	67	180	1.05
31	10	7	1.82	40	13	9	87	0	1.05
27	17	10	1.89	35	22	13	90	0	1.05
24	20	12	1.97	31	26	15	93	180	1.05
32	10	0	1.43	41	13	0	109	0	1.04
24	23	5	1.33	31	30	5	72	180	1.04
27	18	9	1.30	35	23	12	70	180	1.04
32	11	1	1.61	41	14	1	87	180	1.03
25	20	11	1.60	32	26	14	87	0	1.03
31	11	8	1.22	40	14	10	66	180	1.03
24	22	10	2.59	31	28	13	174	0	1.03
27	21	0	1.27	35	27	0	120	180	1.02
28	20	0	1.61	36	26	0	127	0	1.02
24	23	9	1.77	31	30	11	98	0	1.02
24	24	6	1.46	31	31	8	115	180	1.02

33	10	1	1.70	42	13	1	95	0	1.01
28	19	7	1.36	36	24	8	76	0	1.01
32	11	7	1.62	41	14	9	90	0	1.01
28	17	11	1.27	36	22	14	71	180	1.01

Table S16. Prediction of structure factor amplitudes and phases of strong reflections in RHO-G5 from those calculated from the PAU-G3 structure. This is done by converting the reflection indices of RHO-G4 to RHO-G5 according to the relationship below: $h_{\text{RHO-G5}} = h_{\text{RHO-G4}} \times a_{\text{RHO-G5}} / a_{\text{RHO-G4}}$, $k_{\text{RHO-G5}} = k_{\text{RHO-G4}} \times a_{\text{RHO-G5}} / a_{\text{RHO-G4}}$, $l_{\text{RHO-G5}} = l_{\text{RHO-G4}} \times a_{\text{RHO-G5}} / a_{\text{RHO-G4}}$ ($a_{\text{RHO-G4}} = 45 \text{ \AA}$ and $a_{\text{RHO-G5}} = 55 \text{ \AA}$), and then transposing the corresponding structure factor amplitudes and phases of RHO-G4 to RHO-G5. 470 reflections with normalised structure factor $E > 1.2$ and $d > 1.00 \text{ \AA}$ were selected.

$h_{\text{RHO-G4}}$	$k_{\text{RHO-G4}}$	$l_{\text{RHO-G4}}$	E -value	$h_{\text{RHO-G5}}$	$k_{\text{RHO-G5}}$	$l_{\text{RHO-G5}}$	Amplitude	Phase	$d_{\text{PAU-G3}} (\text{\AA})$
4	4	0	2.89	5	5	0	2098	180	7.95
5	4	1	2.83	6	5	1	1028	0	6.94
5	5	0	2.48	6	6	0	1805	180	6.36
8	0	0	1.52	10	0	0	1562	180	5.63
7	4	3	1.25	9	5	4	455	0	5.23
9	1	0	1.64	11	1	0	844	0	4.97
8	4	4	1.86	10	5	5	958	0	4.59
10	0	0	1.62	12	0	0	1660	180	4.50
9	5	4	1.32	11	6	5	478	180	4.07
10	5	5	1.57	12	6	6	805	0	3.67
13	3	2	1.68	16	4	2	426	180	3.34
13	4	1	3.22	16	5	1	815	180	3.30
13	5	0	4.33	16	6	0	1550	0	3.23
14	3	1	1.74	17	4	1	440	0	3.14
13	6	1	1.69	16	7	1	428	0	3.14
14	4	0	4.07	17	5	0	1457	0	3.09
14	5	1	2.97	17	6	1	752	180	3.02
13	7	2	1.24	16	9	3	313	0	3.02
14	6	2	1.29	17	7	2	326	180	2.93
13	8	3	1.33	16	10	4	338	0	2.89
14	7	3	1.24	17	9	4	315	180	2.82
13	8	5	1.85	16	10	6	468	0	2.80
12	10	4	1.29	15	12	5	328	0	2.79
13	9	4	1.57	16	11	5	398	0	2.76
14	8	4	2.73	17	10	5	690	180	2.71
12	11	5	1.49	15	13	6	376	180	2.64
13	10	5	3.01	16	12	6	761	180	2.62
14	9	5	1.49	17	11	6	242	0	2.59
14	10	4	2.18	17	12	5	355	0	2.55
18	0	0	3.52	22	0	0	1619	180	2.50
13	11	6	1.62	16	13	7	262	180	2.49
17	5	4	1.38	21	6	5	223	180	2.48
13	13	0	1.40	16	16	0	454	180	2.45
13	12	7	1.60	16	15	9	260	180	2.37
13	13	8	2.77	16	16	10	496	180	2.24
18	9	1	3.82	22	11	1	483	0	2.23
18	10	0	1.61	22	12	0	288	180	2.19

18	10	2	1.66	22	12	2	210	0	2.18
14	13	9	2.03	17	16	11	257	0	2.13
18	11	1	1.62	22	13	1	205	180	2.13
18	11	3	1.21	23	13	4	152	0	2.11
21	5	0	1.24	26	6	0	222	180	2.08
18	12	2	1.60	22	15	3	202	180	2.07
18	12	4	2.11	22	15	5	267	0	2.05
18	9	9	5.19	22	11	11	927	180	2.04
14	14	10	2.37	17	17	12	388	180	2.03
22	3	1	2.50	27	4	1	290	180	2.02
22	4	0	1.41	27	5	0	232	180	2.01
18	13	3	1.75	22	16	4	203	180	2.01
16	15	5	1.86	20	18	6	216	0	2.00
17	14	5	3.45	21	17	6	400	0	1.99
22	5	1	1.52	27	6	1	176	0	1.99
18	13	5	1.23	22	16	6	143	180	1.98
22	6	2	1.61	27	7	2	186	0	1.97
16	16	4	1.83	20	20	6	300	180	1.96
17	15	4	3.07	21	18	5	356	180	1.95
19	12	5	1.26	23	15	6	146	180	1.95
18	14	4	3.56	22	17	5	413	180	1.94
23	3	0	2.00	28	4	0	328	0	1.94
23	3	2	1.32	28	4	2	153	0	1.93
22	7	3	1.29	27	9	4	149	0	1.93
19	13	4	2.90	23	16	5	336	0	1.93
23	5	0	1.44	28	6	0	236	180	1.91
17	16	3	1.22	21	20	5	141	180	1.91
22	8	4	2.68	27	10	5	311	0	1.89
23	6	1	1.94	28	7	1	226	180	1.89
19	13	6	1.46	23	16	7	170	0	1.89
18	15	5	1.64	22	18	6	190	0	1.88
22	9	5	1.43	27	11	6	252	180	1.85
24	4	0	1.34	29	5	0	335	180	1.85
18	18	0	5.10	22	22	0	1804	0	1.77
17	14	13	2.28	21	17	16	392	180	1.76
23	10	5	1.71	28	12	6	293	0	1.76
18	13	13	2.65	22	16	16	644	0	1.75
26	0	0	3.02	32	0	0	1467	0	1.73
22	14	0	1.34	27	17	0	325	180	1.73
23	13	0	1.24	28	16	0	302	180	1.70
26	4	4	1.38	32	5	5	336	180	1.69
18	14	14	3.12	22	17	17	758	0	1.68
19	14	13	1.84	23	17	16	316	180	1.67
23	14	1	1.37	28	17	1	235	0	1.67
27	1	0	3.29	33	1	0	653	180	1.67
24	13	1	1.54	29	16	1	217	180	1.65

18	18	10	2.32	22	22	12	460	180	1.65
23	15	0	1.36	28	18	0	270	180	1.64
19	18	9	1.48	23	22	11	208	0	1.63
27	5	4	3.20	33	6	5	449	0	1.62
24	14	0	1.27	29	17	0	251	0	1.62
24	14	2	1.23	29	17	2	172	0	1.62
28	0	0	3.04	34	0	0	1205	0	1.61
27	9	0	6.21	33	11	0	942	0	1.58
22	18	4	2.07	27	22	5	222	180	1.57
25	14	3	1.77	31	17	4	189	0	1.56
27	10	1	1.23	33	12	1	131	180	1.56
28	5	5	2.61	34	6	6	396	180	1.56
23	17	4	1.94	28	21	5	208	0	1.56
26	9	9	1.46	32	11	11	221	0	1.55
29	1	0	1.25	35	1	0	190	0	1.55
24	16	4	1.30	29	20	5	140	0	1.55
25	15	0	1.26	31	19	0	190	0	1.54
20	16	14	1.82	24	20	18	195	0	1.54
26	13	3	1.33	32	16	4	143	180	1.54
25	15	4	1.65	31	18	5	177	0	1.53
21	16	13	1.45	26	20	16	155	180	1.53
23	18	5	3.30	28	22	6	300	180	1.52
27	12	3	1.20	33	15	4	109	180	1.52
21	18	11	1.53	26	22	14	139	0	1.51
26	14	4	5.05	32	17	5	459	0	1.51
29	6	5	1.55	35	7	6	141	180	1.50
30	2	0	1.24	37	3	0	159	0	1.50
23	19	4	1.60	28	23	5	145	0	1.50
27	13	4	6.09	33	16	5	553	180	1.49
25	17	0	1.71	31	21	0	219	180	1.49
28	11	3	1.40	34	14	4	127	180	1.49
21	17	14	2.53	26	21	17	230	0	1.48
26	15	5	1.82	32	18	6	166	180	1.48
23	19	6	1.58	28	23	7	143	180	1.48
26	16	0	1.54	32	20	0	198	0	1.47
21	18	13	2.22	26	22	16	201	180	1.47
27	14	3	1.62	33	17	4	148	180	1.47
22	17	13	1.55	27	21	16	200	180	1.47
28	12	4	2.16	34	15	5	278	180	1.46
27	14	5	2.96	33	17	6	382	180	1.46
22	18	12	1.66	27	22	15	214	0	1.46
18	18	18	2.91	22	22	22	918	180	1.44
28	13	5	3.38	34	16	6	436	0	1.44
31	4	1	1.66	38	5	1	215	0	1.44
29	11	4	1.41	35	14	5	181	180	1.44
31	5	0	2.74	38	6	0	499	180	1.43

22	17	15	1.96	27	21	18	252	180	1.42
26	18	0	2.88	32	22	0	524	180	1.42
29	12	5	2.13	35	15	6	208	0	1.42
23	16	15	1.28	28	20	18	125	0	1.42
22	19	13	1.88	27	23	16	183	0	1.41
23	17	14	1.25	28	21	17	121	0	1.41
30	10	4	2.44	37	12	5	238	180	1.41
23	18	13	1.46	28	22	16	142	0	1.41
27	17	2	1.33	33	21	2	129	0	1.41
22	22	8	2.58	27	27	10	356	0	1.40
24	17	13	1.82	29	21	16	178	0	1.40
23	19	12	1.60	28	23	15	156	180	1.40
23	21	8	1.26	28	26	10	123	180	1.40
32	4	0	3.33	39	5	0	459	180	1.40
30	11	5	2.05	37	13	6	199	0	1.39
25	15	14	1.54	31	18	17	150	180	1.39
26	17	9	1.54	32	21	11	150	180	1.39
29	13	6	1.41	35	16	7	137	0	1.39
32	5	1	2.75	39	6	1	268	0	1.39
31	8	5	1.75	38	10	6	171	180	1.39
25	16	13	1.50	32	20	16	146	0	1.39
27	18	1	4.73	33	22	1	461	0	1.39
31	9	4	2.28	38	11	5	222	180	1.38
26	14	14	2.65	32	17	17	449	180	1.38
26	15	13	1.54	32	18	16	185	0	1.38
23	18	15	1.68	28	22	18	201	0	1.37
31	10	5	3.20	38	12	6	383	0	1.37
23	19	14	1.86	28	23	17	222	180	1.37
23	22	9	3.52	28	27	11	422	180	1.36
27	14	13	3.50	33	17	16	419	0	1.36
24	18	14	1.73	29	22	17	207	180	1.36
32	8	4	2.88	39	10	5	344	0	1.35
24	19	13	2.02	29	23	16	242	0	1.35
31	12	1	1.25	38	15	1	150	0	1.35
28	18	0	2.77	34	22	0	469	180	1.35
28	13	13	3.79	34	16	16	641	180	1.34
28	14	12	1.27	34	17	15	152	0	1.34
31	13	0	4.24	38	16	0	569	0	1.34
32	9	5	2.51	39	11	6	238	180	1.34
27	20	1	2.13	33	24	1	202	180	1.34
29	17	0	1.55	35	21	0	208	180	1.34
27	20	3	1.39	33	25	4	132	0	1.33
29	13	12	2.93	35	16	15	278	180	1.32
33	7	4	1.34	40	9	5	127	0	1.32
31	12	7	1.25	38	15	9	119	0	1.32
24	18	16	1.54	29	23	20	146	0	1.32

31	14	1	2.96	38	17	1	281	180	1.32
23	23	10	2.60	28	28	12	349	0	1.32
29	14	11	1.56	36	17	13	148	0	1.32
24	22	10	1.54	29	27	12	146	180	1.32
32	12	2	1.56	39	15	2	148	180	1.31
24	20	14	1.45	29	24	17	137	180	1.31
27	18	11	1.64	33	22	13	156	180	1.31
28	14	14	2.00	34	17	17	269	0	1.31
33	8	5	1.44	40	10	6	136	180	1.31
30	13	11	3.16	37	16	13	330	180	1.30
31	15	2	1.38	38	18	2	131	180	1.30
32	13	1	2.32	39	16	1	242	180	1.30
25	20	13	2.17	32	24	16	226	0	1.30
31	13	8	1.91	38	16	10	200	0	1.30
30	14	10	2.19	37	17	12	228	0	1.30
32	14	0	3.65	39	17	0	539	0	1.29
27	22	3	1.95	33	27	4	204	180	1.29
31	12	11	2.87	38	15	13	299	180	1.29
31	16	3	1.33	38	20	4	139	180	1.29
24	23	11	1.26	29	28	13	131	0	1.29
31	13	10	6.08	38	16	12	634	180	1.28
25	22	11	1.34	32	27	13	140	180	1.28
31	14	9	3.72	38	17	11	389	0	1.28
25	18	17	1.31	31	22	21	137	0	1.28
32	15	1	1.51	39	18	1	175	0	1.27
31	15	8	1.26	38	18	10	146	0	1.27
25	21	14	1.37	31	26	17	158	180	1.27
29	15	14	1.24	35	18	17	143	0	1.27
31	17	4	1.56	38	21	5	181	180	1.26
32	12	10	1.93	39	15	12	223	0	1.26
26	24	4	1.37	32	29	5	159	180	1.26
32	13	9	3.81	39	16	11	441	0	1.26
27	23	4	1.47	33	28	5	170	180	1.26
32	14	8	4.25	39	17	10	492	180	1.26
26	21	13	2.32	32	26	16	268	0	1.25
36	0	0	2.76	44	0	0	905	0	1.25
32	15	7	1.51	39	18	9	174	180	1.25
27	20	13	1.34	34	24	16	155	180	1.25
36	1	1	1.25	44	1	1	204	180	1.25
26	22	12	1.68	32	27	15	195	180	1.25
35	9	0	1.82	43	11	0	247	180	1.25
31	18	5	2.45	38	22	6	235	0	1.24
32	16	6	1.81	39	20	7	174	180	1.24
33	13	8	1.99	40	16	10	191	0	1.24
32	17	3	1.57	39	21	4	150	0	1.24
26	18	18	4.30	32	22	22	584	0	1.24

33	14	7	1.62	40	17	9	156	180	1.23
27	22	11	1.42	34	27	13	136	0	1.23
32	17	5	1.94	39	21	6	186	180	1.23
27	18	17	3.80	33	22	21	365	180	1.23
27	19	16	1.28	33	23	20	123	180	1.23
30	16	14	1.87	37	20	17	180	0	1.22
26	26	0	1.55	32	32	0	297	0	1.22
26	26	2	1.36	32	32	2	184	180	1.22
36	8	0	2.89	44	10	0	392	180	1.22
32	18	4	2.37	39	22	5	242	0	1.22
36	8	2	1.74	44	10	2	178	0	1.22
27	21	14	2.78	33	26	17	285	180	1.22
25	24	13	1.67	31	29	16	171	180	1.22
34	13	7	1.93	43	16	9	197	0	1.21
26	23	13	1.21	32	28	16	124	180	1.21
36	9	1	5.78	44	11	1	591	0	1.21
27	22	13	1.50	33	27	16	153	0	1.21
23	23	18	1.21	28	28	22	175	180	1.21
27	24	9	1.30	34	29	11	132	0	1.21
36	9	3	1.28	45	11	4	131	0	1.21
34	14	6	1.65	42	17	7	168	180	1.21
28	21	13	1.73	34	26	16	176	0	1.21
36	10	0	3.50	44	12	0	507	180	1.20
36	10	2	1.62	44	12	2	165	0	1.20
27	23	12	3.29	33	28	15	336	0	1.20
27	26	1	1.36	33	32	1	139	180	1.20
32	19	5	1.68	39	23	6	172	180	1.20
28	22	12	2.38	34	27	15	243	180	1.20
36	11	1	1.52	44	13	1	188	180	1.20
27	21	16	1.50	34	26	20	185	0	1.19
35	13	6	1.94	43	16	7	239	0	1.19
26	23	15	1.40	32	28	18	173	180	1.19
28	18	18	2.17	34	22	22	378	0	1.19
27	22	15	2.45	33	27	18	303	0	1.19
36	12	2	1.41	37	15	2	174	180	1.18
31	17	14	2.44	38	21	17	301	0	1.18
35	14	5	2.01	43	17	6	248	180	1.18
25	25	14	1.38	31	31	18	240	0	1.18
26	24	14	2.88	32	29	17	355	0	1.18
27	23	14	2.27	33	28	17	280	0	1.18
31	18	13	1.96	38	22	16	241	180	1.18
36	12	4	1.51	44	15	5	186	0	1.18
36	9	9	4.98	44	11	11	869	180	1.18
28	26	0	1.26	34	32	0	219	0	1.18
27	27	2	1.31	33	33	2	228	0	1.18
27	24	13	3.88	33	29	16	304	180	1.17

36	13	3	3.23	44	16	4	253	180	1.17
30	22	10	2.11	37	27	12	166	180	1.17
27	26	9	4.86	33	32	11	381	0	1.17
36	13	5	2.16	44	16	6	170	0	1.17
31	23	0	1.71	38	28	0	190	0	1.17
27	25	12	2.54	34	31	15	199	180	1.16
27	22	17	1.30	34	27	21	102	0	1.16
36	14	4	1.41	44	17	5	111	0	1.16
26	24	16	1.26	33	29	20	98	180	1.16
27	23	16	1.51	34	28	20	118	0	1.16
27	27	8	3.37	33	33	10	374	180	1.15
27	26	11	3.00	33	32	13	235	180	1.15
31	22	9	1.69	38	27	11	133	180	1.15
26	25	15	1.67	33	31	18	152	0	1.15
36	14	6	1.83	44	17	7	166	180	1.15
31	24	1	1.66	38	29	1	151	0	1.15
28	23	15	1.30	34	28	18	118	180	1.15
32	18	14	2.90	39	22	17	263	180	1.15
36	15	5	1.42	44	18	6	129	0	1.14
32	21	9	1.40	39	26	11	127	180	1.14
27	25	14	1.70	34	31	17	155	180	1.14
36	16	0	1.55	44	20	0	199	180	1.14
32	19	13	1.75	39	23	16	159	0	1.14
37	13	4	1.44	45	16	5	131	180	1.14
28	24	14	2.59	34	29	17	235	0	1.14
27	27	10	5.60	33	33	12	719	180	1.14
28	28	0	1.20	34	34	0	218	0	1.14
29	27	0	1.39	35	33	0	178	180	1.14
32	22	8	1.35	39	27	10	123	0	1.13
37	14	3	2.12	45	17	4	193	0	1.13
30	26	2	1.27	38	32	2	104	0	1.13
31	23	10	2.09	38	28	12	172	0	1.13
31	25	2	1.61	39	31	2	132	0	1.13
30	26	4	1.47	37	32	5	121	180	1.13
28	27	9	2.69	34	33	11	222	0	1.13
27	24	17	1.45	34	29	21	119	0	1.13
27	27	12	1.59	34	34	16	186	180	1.12
26	26	16	1.83	32	32	20	214	0	1.12
37	15	4	1.79	45	18	5	147	180	1.12
40	3	1	1.70	49	4	1	140	0	1.12
40	4	0	1.33	49	5	0	154	0	1.12
31	24	9	1.49	38	29	11	123	180	1.12
36	18	0	5.30	44	22	0	617	180	1.12
33	22	7	1.50	40	27	9	124	0	1.12
35	18	9	2.91	43	22	11	239	180	1.11
27	26	15	1.27	34	32	18	104	180	1.11

32	23	9	2.33	39	28	11	132	180	1.11
28	27	11	1.85	34	33	13	105	180	1.11
28	25	15	1.36	35	31	18	112	0	1.11
38	14	2	1.58	47	17	2	90	0	1.11
31	26	3	2.83	38	32	4	161	0	1.11
33	19	14	1.62	40	23	17	92	180	1.11
27	27	14	1.87	34	33	17	151	180	1.11
30	27	5	1.80	37	33	6	102	0	1.11
33	22	9	1.50	40	27	11	85	0	1.11
32	25	3	1.81	39	31	4	103	180	1.11
29	25	14	3.00	36	31	17	171	0	1.10
32	24	8	1.76	39	29	10	100	0	1.10
27	24	19	1.23	34	29	23	70	0	1.10
29	27	10	2.17	35	33	12	123	0	1.10
35	18	11	1.93	43	22	13	110	0	1.10
38	15	1	1.73	47	18	1	98	0	1.10
32	18	18	1.28	40	22	22	103	0	1.10
26	26	18	3.35	32	32	22	269	180	1.10
27	25	18	3.10	33	31	22	177	0	1.10
40	8	4	2.00	49	10	5	114	180	1.10
33	23	8	2.86	40	28	10	181	180	1.10
28	27	13	2.12	35	33	16	121	180	1.10
36	18	8	2.19	44	22	10	139	0	1.10
41	3	0	1.72	50	4	0	154	180	1.09
27	26	17	2.18	33	32	21	138	0	1.09
31	27	2	1.69	39	33	2	107	180	1.09
39	13	2	1.57	48	16	2	99	180	1.09
33	22	11	1.39	40	27	13	88	0	1.09
37	18	1	1.36	45	22	1	86	180	1.09
34	23	3	1.33	42	28	4	84	0	1.09
30	25	13	1.33	37	31	16	84	180	1.09
32	25	7	1.35	40	31	9	86	0	1.09
31	27	4	3.51	38	33	5	222	0	1.09
41	5	0	1.56	50	6	0	140	0	1.09
27	27	16	3.05	33	33	20	273	180	1.09
29	27	12	2.02	36	33	15	128	180	1.09
32	26	4	3.07	39	32	5	194	180	1.09
28	26	16	2.41	34	32	20	152	0	1.09
40	10	4	2.25	49	12	5	143	0	1.09
39	14	1	2.94	48	17	1	186	0	1.09
41	6	1	1.24	50	7	1	79	0	1.09
33	23	10	1.22	40	28	12	77	180	1.09
36	18	10	2.00	44	22	12	127	0	1.09
34	23	7	1.51	43	28	9	96	180	1.08
26	23	23	1.47	32	28	28	158	0	1.08
36	19	9	1.46	44	23	11	111	0	1.08

27	23	22	2.27	33	28	27	173	180	1.08
29	26	15	1.40	36	32	18	106	0	1.08
40	12	0	1.77	49	15	0	191	0	1.08
30	29	5	1.84	37	35	6	140	180	1.07
27	26	19	1.55	33	32	23	118	0	1.07
31	28	5	3.93	38	34	6	299	180	1.07
41	8	5	2.17	50	10	6	165	0	1.07
40	13	1	1.62	49	16	1	123	180	1.07
30	26	14	2.58	37	32	17	196	0	1.07
37	18	9	2.33	45	22	11	178	180	1.07
32	27	5	4.11	39	33	6	313	0	1.07
42	4	0	1.35	51	5	0	145	0	1.07
27	27	18	4.12	33	33	22	443	0	1.07
28	26	18	4.13	34	32	22	235	180	1.07
34	22	12	1.33	42	27	15	76	0	1.07
35	23	6	1.97	43	28	7	112	180	1.06
29	25	18	1.41	35	31	22	80	180	1.06
39	13	10	1.35	48	16	12	77	0	1.06
40	14	0	4.17	49	17	0	336	0	1.06
34	24	8	1.26	43	29	10	72	180	1.06
30	27	13	3.12	37	33	16	177	180	1.06
28	27	17	1.92	34	33	21	109	0	1.06
31	26	13	2.06	38	32	16	117	180	1.06
41	10	5	2.02	50	12	6	115	180	1.06
29	26	17	1.61	35	32	21	92	180	1.06
31	23	18	2.21	38	28	22	126	180	1.06
36	22	6	1.30	44	27	7	74	0	1.06
36	21	9	1.71	45	26	11	97	0	1.06
33	27	2	1.35	41	33	2	77	180	1.05
31	24	17	1.77	38	29	21	101	180	1.05
41	12	1	1.36	50	15	1	77	180	1.05
39	17	4	1.26	48	21	5	72	180	1.05
30	26	16	1.48	38	32	20	84	180	1.05
33	27	4	1.74	40	33	5	108	0	1.05
31	27	12	1.72	38	33	15	107	0	1.05
31	29	6	2.04	38	35	7	127	180	1.05
28	23	23	1.91	34	28	28	168	0	1.05
31	25	16	1.74	39	31	20	108	180	1.05
32	23	17	1.29	39	28	21	80	0	1.05
32	28	6	1.95	39	34	7	121	0	1.05
27	26	21	1.23	34	32	26	77	180	1.05
40	13	9	3.40	49	16	11	212	0	1.05
41	13	0	3.29	50	16	0	290	0	1.05
43	1	0	1.33	53	1	0	117	180	1.05
36	23	5	1.32	44	28	6	82	180	1.05
32	24	16	1.31	39	29	20	82	0	1.04

40	16	0	1.28	50	20	0	113	0	1.04
27	27	20	2.15	33	33	24	189	180	1.04
43	3	0	1.37	54	4	0	121	0	1.04
28	26	20	1.66	34	32	24	103	0	1.04
31	26	15	2.81	38	32	18	175	180	1.04
36	17	17	1.31	44	21	21	115	180	1.04
36	23	7	1.25	45	28	9	78	0	1.04
41	14	1	3.08	50	17	1	192	180	1.04
35	22	13	2.87	43	27	16	179	0	1.04
31	27	14	2.42	38	33	17	147	180	1.04
36	24	4	1.70	44	29	5	103	180	1.04
28	28	18	1.86	34	34	22	159	180	1.03
29	27	18	1.73	35	33	22	105	0	1.03
32	26	14	3.26	39	32	17	197	0	1.03
40	14	10	1.76	49	17	12	107	180	1.03
35	23	12	1.75	43	28	15	106	180	1.03
41	15	0	1.98	50	18	0	170	0	1.03
41	12	9	1.44	50	15	11	87	0	1.03
40	15	9	1.42	49	18	11	86	0	1.03
36	21	13	1.42	44	26	16	86	180	1.03
30	29	13	2.38	37	35	16	144	0	1.03
31	30	7	1.87	38	37	9	113	180	1.03
31	28	13	5.51	38	34	16	333	0	1.03
41	13	8	2.61	50	16	10	158	180	1.03
35	25	8	1.61	43	31	10	98	180	1.03
32	29	7	1.60	40	35	9	97	0	1.03
40	17	5	1.27	49	21	6	77	0	1.03
32	27	13	1.90	39	33	16	115	180	1.03
31	31	0	1.80	38	38	0	217	180	1.03
36	22	12	1.26	44	27	15	76	0	1.03
42	13	1	2.36	51	16	1	172	0	1.02
44	0	0	2.29	54	0	0	473	180	1.02
36	18	18	1.93	44	22	22	199	0	1.02
31	29	12	2.62	38	35	15	191	0	1.02
41	13	10	1.36	50	16	12	99	180	1.02
32	28	12	2.23	39	34	15	163	180	1.02
35	27	0	3.13	43	33	0	323	180	1.02
41	14	9	3.23	50	17	11	236	0	1.02
42	14	0	1.60	51	17	0	165	180	1.02
42	14	2	1.85	51	17	2	135	180	1.02
34	27	9	1.20	42	33	11	87	180	1.01
36	26	0	2.32	44	32	0	239	0	1.01
36	22	14	2.25	44	27	17	139	180	1.01
32	27	15	1.80	39	33	18	112	0	1.01
31	30	11	2.88	38	37	13	178	0	1.01
42	13	7	1.42	51	16	9	88	180	1.01

32	31	1	2.21	39	38	1	137	0	1.01
31	31	8	2.17	38	38	10	190	180	1.01
41	17	4	1.76	50	21	5	109	180	1.01
40	19	5	1.63	49	23	6	101	180	1.01
44	5	5	1.39	54	6	6	121	0	1.01
32	29	11	1.39	40	35	13	86	180	1.01
32	30	8	1.28	39	37	10	79	0	1.01
36	23	13	1.24	44	28	16	77	180	1.01
36	25	9	2.02	44	31	11	125	0	1.01
32	28	14	2.22	39	34	17	137	180	1.01
37	21	14	1.25	45	26	17	77	0	1.00
39	18	13	2.07	48	22	16	128	0	1.00
42	13	9	1.51	51	16	11	93	180	1.00
35	27	8	2.40	43	33	10	148	0	1.00
43	13	0	1.22	54	16	0	106	180	1.00
31	31	10	3.92	38	38	12	342	0	1.00
43	13	2	2.17	54	16	2	134	0	1.00
42	14	8	1.82	51	17	10	113	0	1.00
32	30	10	1.52	39	37	12	94	180	1.00

Table S17. Prediction of structure factor amplitudes and phases of strong reflections in RHO-G6 from those calculated from the RHO-G5 structure. This is done by converting the reflection indices of RHO-G5 to RHO-G6 according to the relationship below: $h_{\text{RHO-G6}} = h_{\text{RHO-G5}} \times a_{\text{RHO-G6}}/a_{\text{RHO-G5}}$, $k_{\text{RHO-G6}} = k_{\text{RHO-G5}} \times a_{\text{RHO-G6}}/a_{\text{RHO-G5}}$, $l_{\text{RHO-G6}} = l_{\text{RHO-G5}} \times a_{\text{RHO-G6}}/a_{\text{RHO-G5}}$ ($a_{\text{RHO-G5}} = 55 \text{ \AA}$ and $a_{\text{RHO-G6}} = 65 \text{ \AA}$), and then transposing the corresponding structure factor amplitudes and phases of RHO-G5 to RHO-G6. 742 reflections with normalised structure factor $E > 1.2$ and $d > 1.00 \text{ \AA}$ were selected.

$h_{\text{RHO-G5}}$	$k_{\text{RHO-G5}}$	$l_{\text{RHO-G5}}$	E -value	$h_{\text{RHO-G6}}$	$k_{\text{RHO-G6}}$	$l_{\text{RHO-G6}}$	Amplitude	Phase	$d_{\text{RHO-G5}} (\text{\AA})$
5	4	1	1.33	6	5	1	663	180	8.49
5	5	0	3.71	6	6	0	3689	180	7.78
6	4	2	1.40	7	5	2	697	0	7.35
6	5	1	3.52	7	6	1	1752	0	6.99
6	6	0	3.23	7	7	0	3208	180	6.48
7	5	2	1.50	8	6	2	747	0	6.23
10	0	0	2.16	12	0	0	3044	180	5.50
11	1	0	2.09	13	1	0	1469	0	4.98
9	5	4	1.35	11	6	5	670	0	4.98
12	0	0	2.22	14	0	0	3118	180	4.58
10	5	5	2.47	12	6	6	1738	0	4.49
11	6	5	1.73	13	7	6	860	180	4.08
12	6	6	1.93	14	7	7	1357	0	3.74
11	11	0	1.35	13	13	0	1341	180	3.54
16	3	3	1.29	24	4	4	610	180	3.32
16	4	2	2.00	19	5	2	667	180	3.31
16	5	1	4.43	19	6	1	1478	180	3.28
16	6	0	5.78	19	7	0	2725	0	3.22
17	3	2	1.26	20	4	2	419	0	3.16
16	7	1	2.22	19	8	1	739	0	3.14
17	4	1	2.19	20	5	1	730	0	3.14
17	5	0	5.38	20	6	0	2535	0	3.10
16	8	2	1.64	19	9	2	546	0	3.06
17	6	1	3.69	20	7	1	1231	180	3.05
17	7	2	1.53	20	8	2	511	180	2.97
16	9	3	1.26	19	11	4	418	0	2.96
18	6	2	1.21	21	7	2	403	180	2.88
16	10	4	1.79	19	12	5	596	0	2.85
17	9	4	1.41	20	11	5	469	180	2.80
14	13	5	1.22	17	15	6	408	0	2.79
16	10	6	2.45	19	12	7	815	0	2.78
15	12	5	1.83	18	14	6	611	0	2.77
16	11	5	2.05	19	13	6	684	0	2.74
17	10	5	3.67	20	12	6	1223	180	2.70
15	13	6	1.54	18	15	7	515	180	2.65
18	9	5	1.20	21	11	6	401	180	2.65
16	12	6	3.84	19	14	7	1280	180	2.63

17	11	6	1.38	20	13	7	461	0	2.60
19	8	5	1.26	23	9	6	259	180	2.59
17	12	5	2.99	20	14	6	615	0	2.57
18	10	6	1.98	21	12	7	408	0	2.56
16	13	7	2.39	19	15	8	491	180	2.53
17	12	7	1.30	20	14	8	268	0	2.51
22	0	0	4.36	26	0	0	2537	180	2.50
21	6	5	2.08	25	7	6	427	180	2.45
16	16	0	1.84	19	19	0	756	180	2.43
16	14	8	1.92	20	17	9	394	180	2.42
22	8	2	1.29	29	9	2	265	180	2.34
16	15	9	1.81	19	18	11	373	180	2.32
24	0	0	1.23	28	0	0	718	0	2.29
24	1	1	1.22	28	1	1	354	180	2.29
22	10	0	1.76	26	12	0	513	180	2.28
22	11	1	4.10	26	13	1	683	0	2.23
16	16	10	3.72	19	19	12	877	180	2.22
17	15	10	1.40	20	18	12	233	0	2.22
22	12	0	2.09	26	14	0	494	180	2.19
22	12	2	2.15	26	14	2	358	0	2.19
22	13	1	1.89	26	15	1	316	180	2.15
16	16	12	1.39	19	19	14	327	0	2.15
17	16	11	2.68	20	19	13	448	0	2.13
17	17	10	1.51	20	20	12	356	0	2.11
22	14	2	1.35	27	17	2	225	180	2.10
26	3	1	1.75	31	4	1	292	180	2.10
22	14	4	1.42	26	17	5	237	0	2.08
26	5	1	1.72	31	6	1	287	0	2.08
26	6	0	1.87	31	7	0	442	180	2.06
22	15	3	1.48	26	18	4	247	180	2.05
17	17	12	2.43	20	20	14	574	180	2.05
18	16	12	1.53	21	19	14	255	0	2.04
22	11	11	6.99	26	13	13	1649	180	2.04
22	15	5	1.98	26	18	6	331	0	2.03
27	3	2	1.58	32	4	2	232	180	2.02
27	4	1	3.50	32	5	1	517	180	2.01
21	17	4	1.88	25	20	5	277	0	2.01
27	5	0	2.16	32	6	0	450	180	2.00
22	16	4	2.52	26	19	5	371	180	2.00
19	19	6	1.21	23	22	7	252	0	2.00
20	18	6	1.88	24	21	7	277	0	2.00
21	17	6	4.06	25	20	7	598	0	1.99
27	6	1	2.57	32	7	1	379	0	1.99
21	18	3	1.63	25	21	4	241	0	1.98
22	16	6	1.90	26	19	7	280	180	1.97
27	7	0	1.24	32	8	0	258	0	1.97

18	17	13	1.87	21	20	15	275	180	1.97
26	9	5	1.52	31	11	6	224	0	1.97
28	0	0	1.31	34	0	0	545	0	1.96
20	19	5	2.27	24	22	6	335	180	1.96
21	18	5	2.64	25	21	6	390	180	1.96
23	15	6	1.27	27	18	7	187	180	1.96
28	3	1	1.43	33	4	1	211	180	1.95
22	17	5	4.39	26	20	6	647	180	1.95
28	4	0	3.01	33	5	0	627	0	1.94
27	8	3	1.54	33	9	4	228	0	1.94
23	16	5	3.04	27	19	6	449	0	1.93
28	5	1	1.38	33	6	1	204	0	1.93
28	6	0	1.98	33	7	0	412	180	1.92
22	17	7	1.27	26	20	8	187	180	1.92
24	15	5	1.27	28	18	6	187	0	1.91
27	9	4	1.41	32	11	5	208	0	1.91
28	7	1	2.71	33	8	1	400	180	1.90
23	16	7	1.68	27	19	8	248	0	1.90
21	20	1	1.35	25	24	1	199	0	1.90
29	1	0	1.72	35	1	0	359	0	1.90
22	18	6	1.20	26	21	7	177	0	1.89
29	3	0	2.13	34	4	0	444	0	1.89
20	16	14	1.33	24	19	17	196	0	1.88
23	17	6	1.73	27	20	7	255	180	1.88
27	10	5	4.06	32	12	6	598	0	1.88
29	5	0	1.75	34	6	0	565	180	1.87
29	6	1	1.54	34	7	1	352	0	1.86
27	11	6	1.67	32	13	7	381	180	1.85
30	2	0	1.48	36	2	0	477	0	1.83
27	12	7	1.21	32	14	8	275	180	1.81
28	11	5	1.30	33	13	6	296	180	1.80
26	16	0	1.27	31	19	0	410	0	1.80
31	1	0	1.50	37	1	0	484	0	1.77
28	12	6	2.16	33	14	7	492	0	1.77
26	17	1	1.69	31	20	1	385	180	1.77
22	22	0	6.95	26	26	0	3169	0	1.77
20	18	16	1.26	24	21	19	286	180	1.76
21	17	16	3.08	25	20	19	682	180	1.75
27	16	1	1.30	32	19	1	287	0	1.75
22	16	16	3.36	26	19	19	1051	0	1.74
27	17	0	1.65	32	20	0	518	180	1.72
32	0	0	3.91	38	0	0	2447	0	1.72
28	16	0	1.44	33	19	0	450	180	1.71
22	17	17	3.58	26	20	20	1122	0	1.69
22	22	10	1.47	26	26	12	461	180	1.68
23	17	16	2.27	27	20	19	503	180	1.68

28	17	1	1.53	33	20	1	338	0	1.68
32	5	5	2.27	38	6	6	710	180	1.68
33	1	0	3.15	39	1	0	987	180	1.67
29	16	1	1.61	34	19	1	357	180	1.66
27	16	11	1.22	32	19	13	185	0	1.65
28	18	0	2.18	33	21	0	469	180	1.65
22	22	12	3.41	26	26	14	733	180	1.65
27	17	10	1.38	32	20	12	210	180	1.64
29	17	0	2.01	34	20	0	432	0	1.64
29	17	2	1.86	34	20	2	283	0	1.63
23	22	11	2.52	27	26	13	383	0	1.63
23	18	17	1.83	27	21	20	278	0	1.63
33	6	5	4.74	39	7	6	720	0	1.62
24	18	16	1.49	28	21	19	226	180	1.62
34	0	0	4.12	40	0	0	1771	0	1.62
30	16	2	1.42	35	19	2	216	180	1.61
34	2	0	1.97	40	2	0	424	180	1.61
23	22	13	1.22	27	26	15	186	180	1.60
30	17	3	1.23	36	20	4	187	0	1.59
29	19	0	1.37	34	22	0	295	180	1.59
33	11	0	7.79	39	13	0	1439	0	1.58
35	1	0	1.55	41	1	0	287	0	1.57
31	16	3	1.72	37	19	4	224	180	1.57
34	6	6	3.15	40	7	7	582	180	1.57
34	7	5	1.39	40	8	6	182	0	1.57
33	12	1	1.58	39	14	1	206	180	1.57
35	3	0	1.29	42	4	0	239	180	1.57
27	22	5	2.88	32	26	6	377	180	1.56
25	19	16	1.28	35	22	19	167	180	1.56
28	21	5	2.63	33	25	6	343	0	1.56
24	22	14	1.34	29	26	17	175	180	1.55
29	20	5	1.27	34	24	6	167	0	1.55
32	11	11	1.93	38	13	13	356	0	1.55
31	17	4	2.11	37	20	5	275	0	1.55
25	22	13	1.32	37	26	15	172	0	1.54
30	19	5	1.43	36	22	6	187	0	1.53
27	23	6	1.69	32	27	7	221	0	1.53
32	16	4	1.82	38	19	5	238	180	1.53
34	12	0	1.49	40	14	0	275	0	1.53
30	20	0	1.51	36	24	0	279	180	1.53
28	22	6	3.74	33	26	7	489	180	1.52
35	7	6	1.83	41	8	7	239	180	1.52
31	18	5	2.38	37	21	6	254	0	1.52
35	8	5	1.21	41	9	6	129	0	1.52
25	20	17	2.00	30	24	20	213	0	1.52
31	19	0	1.55	38	22	0	234	0	1.51

26	20	16	1.48	31	24	19	157	180	1.51
25	22	15	1.88	30	26	18	200	180	1.51
28	23	5	1.93	33	27	6	205	0	1.50
32	17	5	7.73	38	20	6	823	0	1.50
27	24	7	1.27	32	28	8	135	0	1.49
26	22	14	1.45	31	26	17	155	0	1.49
31	19	6	1.59	37	22	7	169	180	1.49
28	23	7	2.34	33	27	8	249	180	1.49
34	14	4	1.27	40	17	5	136	180	1.49
33	16	5	7.90	39	19	6	841	180	1.49
23	21	20	1.50	27	25	24	160	0	1.49
28	24	4	1.37	33	28	5	146	0	1.48
32	18	6	1.85	38	21	7	197	180	1.48
25	21	18	1.52	30	25	21	162	0	1.48
34	11	11	1.48	40	13	13	223	0	1.47
25	22	17	1.26	30	26	20	134	180	1.47
31	21	0	1.71	37	25	0	257	180	1.47
34	15	5	4.17	40	18	6	444	180	1.47
26	21	17	3.00	31	25	20	319	0	1.47
37	6	1	1.47	44	7	1	157	180	1.47
27	26	1	1.30	32	31	1	138	180	1.47
33	17	6	4.29	39	20	7	582	180	1.46
26	22	16	2.70	31	26	19	367	180	1.46
27	25	8	1.33	33	30	9	180	0	1.46
32	20	0	1.76	38	24	0	338	0	1.46
27	21	16	2.48	32	25	19	337	180	1.46
33	18	5	1.31	39	21	6	178	0	1.45
27	22	15	2.23	32	26	18	303	0	1.45
35	14	5	1.78	41	17	6	242	180	1.45
34	16	6	5.16	40	19	7	701	0	1.45
22	22	22	3.19	26	26	26	1061	180	1.44
27	27	0	1.50	32	32	0	407	180	1.44
28	22	14	1.28	33	26	17	174	0	1.44
38	5	1	2.60	45	6	1	353	0	1.43
30	24	0	1.37	36	28	0	263	180	1.43
38	6	0	4.15	45	7	0	798	180	1.43
35	15	6	1.79	41	18	7	243	0	1.43
27	26	9	1.34	32	31	11	183	0	1.43
27	20	19	1.33	32	24	22	181	180	1.42
33	20	1	2.57	39	24	1	349	180	1.42
31	23	0	1.23	37	27	0	237	180	1.42
36	13	5	1.59	43	15	6	216	180	1.42
34	17	7	1.75	40	20	8	238	180	1.42
27	21	18	2.21	32	25	21	300	180	1.42
33	20	3	1.29	40	24	4	175	0	1.42
32	22	0	5.20	38	26	0	1012	180	1.42

27	23	16	2.00	32	27	19	275	0	1.41
28	21	17	1.75	33	25	20	241	0	1.41
36	14	6	1.65	44	17	7	227	0	1.41
35	16	7	1.75	41	19	8	241	0	1.41
33	21	0	1.20	39	25	0	234	0	1.41
33	21	2	1.35	39	25	2	186	0	1.40
28	23	15	1.29	33	27	18	177	180	1.40
29	21	16	1.27	34	25	19	175	0	1.40
37	12	5	2.63	44	14	6	362	180	1.40
39	5	0	3.37	46	6	0	657	180	1.40
34	20	0	2.32	40	24	0	451	0	1.39
39	6	1	1.89	46	7	1	260	0	1.39
27	27	10	3.38	32	32	12	657	0	1.39
28	26	10	1.53	33	31	12	210	180	1.39
39	7	2	1.38	46	8	2	190	0	1.39
33	22	1	4.62	39	26	1	636	0	1.39
37	13	6	1.80	44	15	7	248	0	1.39
31	18	17	1.47	37	21	20	202	180	1.39
31	19	16	1.45	37	22	19	199	0	1.38
38	10	6	1.67	45	12	7	229	180	1.38
32	21	11	1.43	38	25	13	197	180	1.38
35	19	0	1.32	42	22	0	256	0	1.38
38	11	5	2.72	45	13	6	375	180	1.38
28	22	18	2.24	33	26	21	309	0	1.38
28	23	17	2.01	33	27	20	282	180	1.37
32	17	17	3.74	38	20	20	728	180	1.37
32	18	16	1.81	38	21	19	254	0	1.37
38	12	4	1.25	45	14	5	176	0	1.37
29	22	17	1.71	34	26	20	240	180	1.37
36	16	8	1.27	46	19	9	179	0	1.37
33	23	2	1.63	39	27	2	229	0	1.37
38	12	6	3.87	45	14	7	543	0	1.36
29	23	16	2.75	34	27	19	385	0	1.36
33	17	16	5.18	39	20	19	726	0	1.36
28	27	11	4.50	33	32	13	631	180	1.36
34	22	0	4.86	40	26	0	964	180	1.36
38	14	2	1.33	45	17	2	187	0	1.36
39	10	5	3.52	46	12	6	493	0	1.36
32	22	12	1.37	38	26	14	192	0	1.35
38	13	7	1.66	45	15	8	233	0	1.35
33	24	1	1.59	39	28	1	223	180	1.35
34	16	16	4.52	40	19	19	896	180	1.35
34	17	15	2.44	40	20	18	342	0	1.35
38	15	1	2.58	45	18	1	362	0	1.35
32	23	11	1.44	38	27	13	202	180	1.34
33	24	3	1.57	40	28	4	220	0	1.34

39	11	6	2.55	46	13	7	358	180	1.34
29	22	19	1.59	34	26	22	223	0	1.34
38	16	0	5.52	45	19	0	942	0	1.33
38	14	8	1.22	46	17	9	148	0	1.33
35	16	15	3.82	41	19	18	461	180	1.33
40	9	5	1.45	47	11	6	175	0	1.33
37	16	9	1.26	44	19	11	153	0	1.33
30	22	18	1.61	35	26	21	194	180	1.33
35	17	14	1.62	41	20	17	195	0	1.33
28	28	12	3.09	33	33	14	527	0	1.33
29	27	12	2.00	34	32	14	242	180	1.33
32	23	13	2.11	38	27	15	255	0	1.33
33	25	4	1.26	39	30	5	152	0	1.32
30	24	16	1.77	35	28	19	214	0	1.32
34	24	0	1.68	40	28	0	287	0	1.32
34	17	17	2.05	40	20	20	350	0	1.32
38	17	1	3.63	45	20	1	438	180	1.32
40	10	6	1.41	47	12	7	170	180	1.32
33	22	13	1.98	39	26	15	239	180	1.32
36	16	14	3.29	44	19	17	398	180	1.32
39	15	2	1.44	46	18	2	174	180	1.31
38	15	9	1.22	45	18	11	148	0	1.31
35	23	0	1.55	41	27	0	265	180	1.31
36	17	13	1.82	43	20	15	220	0	1.31
42	0	0	1.45	50	0	0	495	180	1.31
42	1	1	1.57	50	1	1	268	0	1.31
38	18	2	1.60	45	21	2	193	180	1.31
33	26	3	1.32	39	31	4	159	180	1.31
39	16	1	3.48	46	19	1	420	180	1.30
36	22	0	1.61	44	26	0	275	180	1.30
33	24	11	1.44	39	28	13	178	0	1.30
33	26	5	2.01	39	31	6	249	0	1.30
37	16	13	2.97	44	19	15	368	180	1.30
38	16	10	2.16	45	19	12	267	0	1.30
37	17	12	2.55	44	20	14	316	0	1.30
34	23	11	1.40	40	27	13	174	180	1.29
36	16	16	1.42	44	19	19	249	180	1.29
39	17	0	4.49	46	20	0	787	0	1.29
38	19	3	1.75	46	22	4	217	180	1.29
32	28	4	1.21	38	33	5	149	0	1.29
33	27	4	1.99	39	32	5	246	180	1.28
38	14	14	2.24	46	17	17	391	180	1.28
35	18	17	1.42	41	21	20	176	0	1.28
38	15	13	3.16	45	18	15	391	180	1.28
31	25	16	1.64	37	30	19	203	0	1.28
38	16	12	8.36	45	19	14	1034	180	1.28

39	18	1	2.21	46	21	1	273	0	1.28
35	25	0	1.33	42	30	0	232	0	1.28
34	23	13	1.38	40	27	15	171	0	1.28
38	17	11	4.71	45	20	13	583	0	1.28
43	2	1	1.20	51	2	1	149	180	1.28
38	18	10	2.45	45	21	12	303	0	1.27
32	25	15	1.42	38	30	18	189	0	1.27
34	24	12	1.26	40	28	14	169	180	1.27
33	28	3	1.31	39	33	4	175	180	1.27
39	14	13	1.21	46	17	15	161	0	1.27
42	11	1	1.74	50	13	1	233	180	1.27
31	22	21	1.23	37	26	25	164	0	1.27
31	27	14	1.20	37	32	17	161	180	1.27
39	15	12	2.37	46	18	14	316	0	1.27
32	29	5	2.04	38	34	6	272	180	1.27
39	16	11	4.78	46	19	13	638	0	1.26
33	28	5	1.59	39	33	6	212	180	1.26
38	20	8	1.40	45	24	9	187	0	1.26
32	22	20	1.56	38	26	24	208	180	1.26
39	17	10	5.76	46	20	12	769	180	1.26
34	27	5	1.34	40	32	6	179	0	1.26
38	21	5	3.14	45	25	6	419	180	1.26
43	6	5	1.55	51	7	6	207	0	1.26
40	18	0	1.20	47	21	0	227	0	1.25
39	18	9	1.92	46	21	11	257	180	1.25
38	22	0	1.22	46	26	0	230	180	1.25
44	0	0	3.61	52	0	0	1363	0	1.25
44	1	1	1.20	52	1	1	226	180	1.25
39	17	12	1.40	46	20	14	154	0	1.24
40	16	10	2.80	47	19	12	310	0	1.24
32	26	16	3.07	38	31	19	340	0	1.24
38	22	6	3.45	45	26	7	382	0	1.24
40	17	9	2.17	47	20	11	241	180	1.24
43	11	0	1.88	51	13	0	295	180	1.24
33	25	16	1.66	39	30	19	184	180	1.24
31	23	22	1.74	37	27	26	193	0	1.24
39	21	4	1.82	46	25	5	202	0	1.24
32	27	15	2.70	38	32	18	299	180	1.24
44	5	5	1.46	52	6	6	229	180	1.23
40	18	8	1.20	48	21	9	133	180	1.23
32	22	22	4.36	38	26	26	682	0	1.23
32	31	3	1.32	39	37	4	146	180	1.23
39	21	6	2.64	46	25	7	292	180	1.23
38	23	5	1.55	45	27	6	172	180	1.23
42	11	11	1.32	50	13	13	206	0	1.23
33	22	21	4.30	39	26	25	476	180	1.23

41	16	9	2.37	48	19	11	262	0	1.22
44	9	1	2.39	52	11	1	265	180	1.22
34	29	5	1.59	40	34	6	176	180	1.22
45	1	0	1.49	53	1	0	234	0	1.22
33	24	19	1.32	40	28	22	146	180	1.22
34	26	14	1.22	40	31	17	136	180	1.22
39	22	5	3.91	46	26	6	433	0	1.22
41	17	8	1.41	49	20	9	156	180	1.22
44	10	0	3.51	52	12	0	550	180	1.22
33	25	18	2.23	39	30	21	247	180	1.22
34	22	20	1.93	40	26	24	236	180	1.22
44	10	2	1.51	52	12	2	168	0	1.22
32	32	0	1.32	38	38	0	322	0	1.22
33	31	0	1.40	39	37	0	241	180	1.21
36	23	15	1.39	43	27	18	170	0	1.21
28	28	22	1.41	33	33	26	244	180	1.21
32	32	2	1.45	38	38	2	250	180	1.21
33	26	17	4.21	39	31	20	513	180	1.21
30	30	16	1.35	36	35	19	233	180	1.21
44	11	1	7.22	52	13	1	882	0	1.21
31	29	16	1.55	37	34	19	189	180	1.21
32	28	16	1.79	38	33	19	218	180	1.21
39	23	4	1.28	46	27	5	157	0	1.21
40	21	5	1.26	47	25	6	154	180	1.21
33	27	16	1.62	39	32	19	197	0	1.21
44	12	0	4.3	52	14	0	743	180	1.21
44	12	2	1.95	52	14	2	238	0	1.20
42	16	8	1.40	50	19	9	171	0	1.20
39	23	6	2.39	46	27	7	291	180	1.20
34	26	16	3.14	40	31	19	383	0	1.20
33	28	15	3.65	39	33	18	446	0	1.20
37	27	0	1.61	44	32	0	278	0	1.20
42	17	7	1.25	50	20	8	152	180	1.20
44	13	1	2.26	52	15	1	276	180	1.20
34	27	15	2.40	40	32	18	293	180	1.20
43	15	6	2.05	51	18	7	250	180	1.20
33	32	1	1.96	39	38	1	239	180	1.20
44	13	3	1.35	53	15	4	165	0	1.20
33	25	20	1.27	40	30	24	155	0	1.20
38	26	0	1.89	45	31	0	327	180	1.19
34	22	22	2.28	40	26	26	434	0	1.19
33	29	14	2.41	39	34	17	324	0	1.19
32	28	18	2.23	38	33	21	301	180	1.19
44	14	2	1.40	53	17	2	188	180	1.19
33	27	18	2.74	39	32	21	369	0	1.19
44	14	4	1.34	52	17	5	181	0	1.19

31	30	17	1.95	37	35	20	263	0	1.19
33	31	10	1.22	39	37	12	165	0	1.19
32	29	17	3.56	38	34	20	480	0	1.19
43	16	7	1.73	51	19	8	234	0	1.19
33	30	13	1.63	40	35	15	219	0	1.18
33	28	17	2.64	39	33	20	356	0	1.18
38	20	18	1.73	45	24	21	233	0	1.18
44	15	3	1.31	52	18	4	176	180	1.18
34	27	17	1.21	40	32	20	163	180	1.18
43	17	6	2.80	51	20	7	377	180	1.18
38	21	17	2.71	45	25	20	365	0	1.18
44	11	11	6.80	52	13	13	1297	180	1.18
34	32	0	1.90	40	38	0	363	0	1.18
33	33	2	1.86	39	39	2	355	0	1.18
34	32	2	1.82	40	38	2	246	180	1.18
38	22	16	2.13	45	26	19	287	180	1.18
33	29	16	3.32	39	34	19	447	180	1.18
44	15	5	2.48	52	18	6	334	0	1.18
35	26	17	1.49	41	31	20	201	180	1.18
33	31	12	2.65	39	37	14	357	0	1.17
44	16	4	3.64	52	19	5	293	180	1.17
47	1	0	1.44	57	1	0	164	180	1.17
33	30	15	2.60	39	35	18	210	180	1.17
34	24	22	1.59	40	28	26	128	180	1.17
36	28	12	1.86	43	33	14	150	180	1.17
32	29	19	2.02	38	34	22	163	180	1.17
40	25	1	1.31	47	30	1	106	0	1.17
44	16	6	2.61	52	19	7	210	0	1.17
38	28	0	1.40	45	33	0	160	0	1.17
33	28	19	1.74	39	33	22	140	0	1.16
44	17	3	1.32	52	20	4	106	180	1.16
33	32	11	6.37	39	38	13	513	0	1.16
35	23	22	1.21	41	27	26	98	0	1.16
37	27	12	3.74	44	32	14	301	180	1.16
34	33	1	1.29	40	39	1	104	180	1.16
35	30	11	1.30	42	35	13	105	0	1.16
39	25	10	1.23	46	30	12	99	0	1.16
41	22	9	1.73	49	26	11	139	180	1.16
33	31	14	1.73	40	37	17	139	180	1.16
32	30	18	2.15	38	35	21	173	0	1.16
44	17	5	2.00	52	20	6	161	0	1.16
36	29	11	1.38	43	34	13	111	0	1.16
35	32	3	1.51	42	38	4	121	180	1.16
34	28	18	2.35	40	33	21	189	180	1.16
38	26	12	2.02	45	31	14	163	0	1.16
36	22	22	1.29	44	26	26	146	0	1.16

44	17	7	2.42	52	20	8	195	180	1.15
37	28	11	2.21	44	33	13	178	0	1.15
33	30	17	2.10	39	35	20	169	180	1.15
33	33	10	4.27	39	39	12	486	180	1.15
33	32	13	1.51	39	38	15	143	180	1.15
34	29	17	4.11	40	34	20	389	0	1.15
38	29	1	2.65	45	34	1	250	0	1.15
43	21	0	1.70	51	25	0	227	0	1.15
39	22	17	3.75	46	26	20	355	180	1.15
38	27	11	1.95	45	32	13	185	180	1.15
44	18	6	1.97	52	21	7	187	0	1.15
45	16	5	1.70	53	19	6	161	180	1.15
39	23	16	1.42	46	27	19	135	0	1.15
33	31	16	1.22	40	37	19	115	180	1.15
34	34	0	1.86	40	40	0	352	0	1.14
35	33	0	1.29	41	39	0	173	180	1.14
34	34	2	1.71	40	40	2	229	180	1.14
39	26	11	1.71	46	31	13	162	180	1.14
33	33	12	6.97	39	39	14	932	180	1.14
44	18	8	1.41	52	21	9	133	180	1.14
32	30	20	1.79	39	35	24	170	180	1.14
38	28	10	1.34	45	33	12	127	180	1.14
45	17	4	2.99	53	20	5	283	0	1.14
45	16	7	1.40	53	19	8	132	0	1.14
35	33	4	1.33	42	39	5	126	0	1.14
41	22	13	1.52	49	26	15	144	180	1.14
48	6	0	1.28	57	7	0	172	0	1.14
32	31	19	1.59	39	37	22	151	0	1.14
38	30	2	1.38	45	35	2	131	0	1.14
39	27	10	1.92	46	32	12	182	0	1.13
45	18	3	1.32	53	21	4	125	0	1.13
39	29	0	1.72	46	34	0	195	180	1.13
34	33	11	3.57	40	39	13	286	0	1.13
38	29	9	1.53	45	34	11	122	180	1.13
38	28	12	3.06	45	33	14	245	0	1.13
45	18	5	2.37	53	21	6	190	180	1.13
33	33	14	1.56	40	39	17	177	180	1.13
33	31	18	1.43	40	37	21	115	180	1.13
34	30	18	2.16	40	35	21	173	0	1.13
40	28	0	1.51	47	33	0	171	0	1.13
46	16	4	1.50	54	19	5	120	180	1.13
35	34	3	1.38	42	40	4	110	180	1.13
38	29	11	2.43	45	34	13	195	180	1.12
38	30	8	1.84	46	35	9	147	180	1.12
35	30	17	1.49	41	35	20	119	0	1.12
46	17	3	1.81	54	20	4	145	0	1.12

34	33	13	2.53	40	39	15	202	180	1.12
49	3	2	1.45	58	4	2	116	0	1.12
38	31	3	2.96	45	37	4	237	0	1.12
40	23	17	2.16	47	27	20	173	180	1.12
49	4	1	2.28	58	5	1	182	0	1.12
37	32	5	1.93	44	38	6	154	180	1.12
44	22	0	6.53	52	26	0	739	180	1.12
44	22	2	1.35	52	26	2	108	0	1.12
39	28	11	1.84	46	33	13	147	180	1.12
45	20	1	1.48	53	24	1	118	0	1.12
49	5	0	1.57	58	6	0	178	0	1.12
32	31	21	1.43	38	37	25	114	180	1.12
33	30	21	1.70	40	35	25	136	0	1.12
40	24	16	1.46	47	28	19	117	0	1.12
49	6	1	1.37	58	7	1	86	180	1.11
46	18	2	1.25	55	21	2	79	0	1.11
41	27	6	1.30	49	32	7	82	180	1.11
32	32	20	2.36	38	38	24	211	0	1.11
40	27	11	2.80	47	32	13	177	0	1.11
49	7	0	1.68	58	8	0	150	180	1.11
49	7	2	1.40	58	8	2	89	180	1.11
43	22	11	5.13	51	26	13	324	180	1.11
38	31	7	1.24	45	37	8	78	180	1.11
36	26	22	1.28	43	31	26	81	180	1.11
35	33	12	2.05	41	39	14	129	0	1.11
39	29	10	3.02	46	34	12	191	0	1.11
45	21	0	1.44	53	25	0	129	0	1.11
34	33	15	1.72	41	39	18	108	180	1.11
41	27	8	1.26	49	32	9	80	0	1.11
33	32	19	1.56	40	38	22	99	180	1.11
47	16	3	1.65	57	19	4	104	180	1.11
46	19	1	1.62	55	22	1	102	0	1.10
34	31	19	1.79	41	37	22	113	0	1.10
32	27	27	1.90	38	32	32	169	0	1.10
39	31	0	1.38	47	37	0	123	180	1.10
40	28	10	3.35	47	33	12	211	180	1.10
38	32	4	4.28	45	38	5	270	0	1.10
38	31	9	1.38	46	37	11	87	180	1.10
32	29	25	1.23	38	34	30	78	180	1.10
40	27	13	1.50	47	32	15	94	0	1.10
33	28	25	1.29	39	33	30	81	0	1.10
47	17	0	2.73	56	20	0	244	180	1.10
40	30	0	1.37	47	35	0	123	180	1.10
32	30	24	1.71	39	35	28	108	180	1.10
47	17	2	1.37	56	20	2	86	0	1.10
49	10	1	1.21	59	12	1	76	0	1.10

34	26	26	1.68	40	31	31	150	180	1.10
45	22	1	2.95	53	26	1	186	180	1.10
35	33	14	2.56	42	39	17	161	180	1.10
50	4	0	2.03	59	5	0	213	180	1.10
33	30	23	1.65	40	35	27	122	0	1.10
44	22	10	2.21	52	26	12	164	0	1.10
49	10	5	2.38	58	12	6	177	180	1.09
40	28	12	1.80	47	33	14	134	180	1.09
32	32	22	3.63	38	38	26	381	180	1.09
33	31	22	2.21	39	37	26	164	0	1.09
47	18	1	1.26	56	21	1	94	0	1.09
34	33	17	1.29	41	39	20	96	180	1.09
50	6	0	1.48	59	7	0	155	0	1.09
36	31	17	2.36	43	37	20	175	0	1.09
49	10	7	1.66	58	12	8	123	180	1.09
43	26	5	1.39	51	31	6	103	0	1.09
33	32	21	1.91	39	38	25	142	0	1.09
38	33	5	4.50	45	39	6	334	0	1.09
48	16	0	3.09	57	19	0	324	180	1.09
44	22	12	1.95	52	26	14	145	0	1.09
48	16	2	1.75	57	19	2	130	180	1.09
39	32	5	4.87	46	38	6	361	180	1.08
49	12	5	2.59	58	14	6	192	0	1.08
33	33	20	4.23	39	39	24	444	180	1.08
34	32	20	3.12	40	38	24	231	0	1.08
44	23	11	3.18	52	27	13	236	0	1.08
47	16	11	1.44	56	19	13	107	180	1.08
45	22	9	1.22	53	26	11	108	0	1.08
32	28	28	2.36	38	33	33	293	0	1.08
48	17	1	3.89	57	20	1	342	0	1.08
38	30	16	1.25	46	35	19	110	0	1.08
33	28	27	4.09	39	33	32	360	180	1.08
34	33	19	1.45	41	39	22	128	180	1.08
51	3	0	1.48	60	4	0	185	180	1.08
35	32	19	1.43	42	38	22	126	0	1.08
36	33	15	1.95	43	39	18	172	180	1.08
34	27	27	1.39	40	32	32	174	0	1.08
34	28	26	1.90	40	33	31	167	180	1.08
38	34	4	1.47	45	40	5	129	0	1.08
51	5	0	1.21	60	6	0	151	0	1.07
39	33	4	2.01	46	39	5	177	180	1.07
49	15	0	1.47	58	18	0	182	0	1.07
45	22	11	2.56	53	26	13	225	180	1.07
37	35	6	1.54	44	41	7	136	180	1.07
38	34	6	4.73	45	40	7	416	180	1.07
50	10	6	2.69	59	12	7	236	0	1.07

35	33	18	1.20	42	39	21	106	180	1.07
33	32	23	1.80	39	38	27	158	0	1.07
36	32	18	1.91	43	38	21	168	0	1.07
39	33	6	4.91	46	39	7	432	0	1.07
49	16	1	2.16	58	19	1	190	180	1.07
33	33	22	5.60	39	39	26	696	0	1.07
34	32	22	4.45	40	38	26	303	180	1.07
36	33	17	1.40	43	39	20	95	180	1.06
45	22	13	1.36	53	26	15	93	0	1.06
50	12	6	1.78	59	14	7	121	180	1.06
43	28	7	1.72	51	33	8	117	180	1.06
37	32	17	2.84	44	38	20	193	0	1.06
34	33	21	2.20	40	39	25	150	0	1.06
35	32	21	1.71	41	38	25	116	180	1.06
49	17	0	4.97	58	20	0	477	0	1.06
46	22	10	1.21	54	26	12	82	180	1.06
38	27	23	1.20	45	32	27	82	0	1.06
48	16	12	3.22	57	19	14	219	0	1.06
48	20	2	1.54	58	24	2	104	180	1.06
34	34	20	2.35	40	40	24	226	0	1.06
38	28	22	2.20	45	33	26	150	180	1.06
40	33	5	1.38	47	39	6	94	0	1.06
37	33	16	3.03	44	39	19	206	180	1.06
48	17	11	2.21	57	20	13	151	180	1.06
38	35	7	2.88	45	41	8	196	180	1.05
42	27	15	1.35	50	32	18	92	0	1.05
52	4	0	1.34	61	5	0	129	0	1.05
36	32	20	1.49	44	38	24	101	180	1.05
34	28	28	2.00	40	33	33	192	0	1.05
38	32	16	3.05	45	38	19	207	180	1.05
39	34	7	2.45	46	40	8	166	0	1.05
38	29	21	2.41	45	34	25	164	180	1.05
50	15	1	2.18	59	18	1	148	180	1.05
43	29	6	2.13	51	34	7	145	0	1.05
49	18	1	1.22	58	21	1	83	180	1.05
33	31	26	1.29	40	37	31	88	180	1.05
42	22	22	1.43	50	26	26	137	180	1.05
40	33	7	1.49	47	39	8	87	0	1.05
33	32	25	1.37	40	38	30	80	180	1.05
52	6	2	1.57	61	7	2	91	180	1.05
38	30	20	1.51	45	35	24	88	180	1.05
42	28	14	1.29	50	33	17	75	180	1.05
39	28	21	2.16	46	33	25	125	0	1.05
39	35	0	1.21	47	41	0	100	180	1.05
33	33	24	2.07	39	39	28	170	180	1.05
34	32	24	1.54	40	38	28	90	0	1.05

50	16	0	4.00	59	19	0	328	0	1.05
44	28	6	2.02	52	33	7	117	180	1.05
38	33	15	2.60	45	39	18	151	0	1.05
48	17	13	1.37	57	20	15	79	180	1.05
38	31	19	2.60	45	37	22	151	180	1.05
51	12	5	1.28	60	14	6	74	0	1.05
45	27	4	1.56	53	32	5	90	180	1.05
34	33	23	2.30	40	39	27	134	0	1.04
47	23	6	1.25	56	27	7	73	0	1.04
41	33	2	1.37	49	39	2	79	180	1.04
36	34	18	1.22	43	40	21	71	0	1.04
35	32	23	1.98	41	38	27	115	180	1.04
49	16	11	4.47	58	19	13	259	0	1.04
44	27	11	1.64	53	32	13	95	0	1.04
42	32	0	1.38	50	38	0	113	180	1.04
50	17	1	3.06	59	20	1	178	180	1.04
38	32	18	4.41	45	38	21	256	180	1.04
34	34	22	2.24	40	40	26	184	180	1.04
35	33	22	2.58	41	39	26	150	0	1.04
51	14	1	1.59	60	17	1	92	180	1.04
44	29	5	1.82	52	34	6	106	180	1.04
38	36	8	3.12	46	43	9	181	180	1.04
50	15	9	1.56	59	18	11	91	180	1.04
39	31	18	1.28	46	37	21	74	0	1.04
44	26	14	1.30	52	31	17	75	0	1.04
52	9	5	1.34	61	11	6	85	180	1.04
53	1	0	1.66	63	1	0	149	180	1.04
44	21	21	1.61	52	25	25	145	180	1.04
39	36	1	1.36	46	43	1	86	180	1.04
40	34	8	1.51	47	40	9	96	0	1.04
38	33	17	3.30	45	39	20	210	180	1.04
45	26	11	1.34	54	31	13	85	0	1.04
50	18	0	3.18	59	21	0	286	0	1.03
39	32	17	4.19	46	38	20	266	0	1.03
49	17	12	2.98	58	20	14	189	180	1.03
43	27	16	4.75	51	32	19	302	0	1.03
37	36	13	1.20	44	43	15	76	180	1.03
44	30	2	1.40	53	35	2	89	0	1.03
50	15	11	1.35	59	18	13	86	0	1.03
49	18	11	1.28	58	21	13	81	0	1.03
36	36	16	1.36	44	43	19	122	0	1.03
37	35	16	2.72	44	41	19	173	0	1.03
40	31	17	1.69	47	37	20	108	0	1.03
38	34	16	6.39	45	40	19	405	0	1.03
50	16	10	3.09	59	19	12	196	180	1.03
51	16	1	3.86	60	19	1	245	0	1.03

45	28	7	1.70	53	33	8	108	180	1.03
43	28	15	2.07	51	33	18	131	180	1.03
39	33	16	2.68	46	39	19	170	180	1.03
44	26	16	1.49	52	31	19	95	180	1.03
49	21	6	2.07	58	25	7	131	0	1.03
43	29	14	1.20	51	34	17	83	180	1.02
38	38	0	2.73	45	45	0	380	180	1.02
51	17	0	2.12	60	20	0	209	180	1.02
44	27	15	2.46	52	32	18	171	0	1.02
51	17	2	1.98	60	20	2	138	180	1.02
38	35	15	3.17	45	41	18	221	0	1.02
50	15	13	1.38	59	18	15	96	180	1.02
38	37	9	1.48	45	44	11	103	180	1.02
39	34	15	2.96	46	40	18	206	180	1.02
44	22	22	2.79	52	26	26	275	0	1.02
44	23	21	1.68	52	27	25	117	180	1.02
44	31	3	1.28	55	37	4	89	180	1.02
50	17	11	3.58	59	20	13	250	0	1.02
43	31	10	2.01	51	37	12	140	180	1.02
54	0	0	2.88	64	0	0	567	180	1.02
51	14	11	1.37	60	17	13	95	0	1.02
47	22	15	1.63	56	26	18	114	0	1.02
42	34	0	1.39	50	40	0	137	180	1.02
39	33	18	1.40	46	39	21	98	0	1.02
38	36	14	2.30	46	43	17	160	0	1.02
51	16	9	1.94	60	19	11	136	180	1.01
43	33	0	3.15	51	39	0	311	180	1.01
39	35	14	1.21	46	41	17	84	180	1.01
43	29	16	1.89	51	34	19	132	0	1.01
44	27	17	2.46	52	32	20	142	180	1.01
43	31	12	1.92	51	37	14	111	180	1.01
41	34	11	1.32	49	40	13	76	180	1.01
49	19	14	1.24	59	22	17	71	180	1.01
44	32	0	4.67	52	38	0	381	0	1.01
51	19	0	2.17	60	22	0	177	0	1.01
52	16	2	2.23	61	19	2	129	0	1.01
39	34	17	3.94	46	40	20	228	180	1.01
39	38	1	3.31	46	45	1	191	0	1.01
50	21	5	1.83	59	25	6	105	180	1.01
54	5	5	2.24	64	6	6	183	0	1.01
42	33	11	2.09	50	39	13	121	180	1.01
47	21	18	1.41	56	25	21	81	180	1.01
44	28	16	2.02	52	33	19	116	180	1.01
51	16	11	1.50	60	19	13	86	180	1.01
36	30	28	1.25	44	35	33	72	0	1.01
38	37	13	3.59	45	44	15	207	0	1.01

50	22	0	1.46	60	26	0	119	0	1.01
39	36	13	1.44	46	43	15	83	180	1.01
38	38	10	3.34	45	45	12	272	180	1.01
51	17	10	2.46	60	20	12	142	0	1.01
45	26	17	2.08	53	31	20	120	0	1.01
39	37	10	1.86	46	44	12	107	0	1.01
52	13	11	1.46	62	15	13	84	0	1.01
40	36	10	1.31	47	43	12	76	0	1.00
38	36	16	1.65	46	43	19	95	0	1.00
52	17	3	1.60	62	20	4	92	180	1.00
43	34	1	1.54	51	40	1	89	180	1.00
40	34	16	1.53	47	40	19	88	0	1.00
44	26	20	1.23	53	31	24	71	0	1.00
44	31	11	3.10	52	37	13	179	0	1.00
52	17	5	1.43	62	20	6	83	0	1.00

References

42. Lewis, D. W., Freeman, C. M. & Catlow, C. R. A. Predicting the templating ability of organic additives for the synthesis of microporous materials. *J. Phys. Chem.* **99**, 11194-11202 (1995).
43. Stevens, A. P., Gorman, A. M., Freeman, C. M. & Cox, P. A. Prediction of template location via a combined Monte Carlo-simulated annealing approach. *J. Chem. Soc. Faraday Trans.* **92**, 2065-2073 (1996).
44. Chen, C. Y. *et al.* SSZ-42: the first high-silica large pore zeolite with an undulating, one-dimensional channel system. *Chem. Commun.* 1775-1776, (1997).
45. *Materials Studio software 6.0* Accelrys Inc. (2012).
46. A. Barrett, P., Valencia, S. & A. Cambor, M. Synthesis of a merlinoite-type zeolite with an enhanced Si/Al ratioviapore filling with tetraethylammonium cations. *J. Mater. Chem.* **8**, 2263-2268, (1998).
47. Kim, D. J., Shin, C.-H. & Hong, S. B. Synthesis and characterization of a gallosilicate analog of zeolite paulingite. *Microporous Mesoporous Mater.* **83**, 319-325 (2005).
48. Castro, M. *et al.* Co-templating and modelling in the rational synthesis of zeolitic solids. *Chem. Commun.*, 3470-3472, (2007).
49. Lapshin, A. E., Magdysyuk, O. V., Golubeva, O. Yu. & Nikolaeva, E. A. Distribution of extraframework cations and water molecules in the structure of synthetic paulingite. *Glass Phy. Chem* **37**, 72-77, (2011).