

Supplementary data

Crystal structure data for the refined zeolites

Atomic parameters of the refined structures, parameters of the zeolite framework atoms were not refined and adopted from Mortier *et al.* (1976) and Snellings *et al.* (2009). Parameters fixed during refinement are in italic. SG stands for space group. In the mordenite refinements Ca²⁺ was kept as generic extraframework cation.

A

clinoptilolite

Winston, New Mexico, USA

SG C2/m

a (Å) 17.6697 (9)

b (Å) 17.9321 (10)

c (Å) 7.4116 (3)

β (°) 116.345 (4)

V (Å³) 2104.5 (2)

Site	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>B</i> _{iso}
T1	0.1777	0.1687	0.0926	Si 1.0	1.58
T2	0.2129	0.4113	0.4997	Si 1.0	1.82
T3	0.2107	0.1905	0.7141	Si 1.0	1.73
T4	0.0696	0.298	0.4182	Si 1.0	1.58
T5	0.0	0.2203	0.0	Si 1.0	2.29
O1	0.2021	0.5	0.461	O 1.0	0.79
O2	0.2324	0.1225	0.61	O 1.0	2.61
O3	0.1836	0.1553	0.878	O 1.0	3.95
O4	0.2375	0.1135	0.26	O 1.0	4.66
O5	0.0	0.3225	0.5	O 1.0	4.26
O6	0.0803	0.1667	0.057	O 1.0	1.34
O7	0.126	0.2325	0.56	O 1.0	2.29
O8	0.0097	0.2708	0.189	O 1.0	1.73
O9	0.2141	0.2486	0.183	O 1.0	3.87
O10	0.1203	0.3719	0.414	O 1.0	3.32
M1	0.146 (2)	0.0	0.666 (4)	Na 0.209 (3) Ca 0.135	3.2 (9)
M2	0.034 (2)	0.5	0.21217	Ca 0.384 (7)	8.1 (11)
M3	0.242 (2)	0.5	0.08345	K 0.31 (3)	6.6 (12)
M4	0.0	0.0	0.5	Mg 0.46 (4)	9.5 (15)
W1	0.308 (2)	0.0	0.08523	O 0.62 (2)	2.0 (7)
W3	0.0756 (9)	0.42003	0.96901	O 0.91 (3)	6.0 (13)
W4	0.5	0.0	0.5	O 0.98 (3)	7.4 (11)
W5	0.014 (4)	0.094 (2)	0.397 (7)	O 0.49 (2)	10.8 (16)
W6	0.053 (2)	0.0	0.290 (4)	O 0.64 (4)	12.5 (14)
W7	0.107 (5)	0.0	0.757 (10)	O 0.58 (4)	12.6 (12)
W8	0.066 (4)	0.0	0.063 (9)	O 0.58 (3)	5.6 (7)

B

clinoptilolite

Bowie, Arizona, USA

SG C2/m

a (Å) 17.6694 (13)

b (Å) 17.9488 (14)

c (Å) 7.4116 (4)

 β (°) 116.31 (6)V (Å³) 2107.0 (3)

Site	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>B</i> _{iso}
T1	0.1777	0.1687	0.0926	Si 1.0	1.58
T2	0.2129	0.4113	0.4997	Si 1.0	1.82
T3	0.2107	0.1905	0.7141	Si 1.0	1.73
T4	0.0696	0.298	0.4182	Si 1.0	1.58
T5	0.0	0.2203	0.0	Si 1.0	2.29
O1	0.2021	0.5	0.461	O 1.0	0.79
O2	0.2324	0.1225	0.61	O 1.0	2.61
O3	0.1836	0.1553	0.878	O 1.0	3.95
O4	0.2375	0.1135	0.26	O 1.0	4.66
O5	0.0	0.3225	0.5	O 1.0	4.26
O6	0.0803	0.1667	0.057	O 1.0	1.34
O7	0.126	0.2325	0.56	O 1.0	2.29
O8	0.0097	0.2708	0.189	O 1.0	1.73
O9	0.2141	0.2486	0.183	O 1.0	3.87
O10	0.1203	0.3719	0.414	O 1.0	3.32
M1	0.149 (2)	0.0	0.654 (6)	Na 0.259 (4) Ca 0.135	2.5 (15)
M2	0.033 (2)	0.5	0.197 (4)	Ca 0.361 (7)	7.3 (15)
M3	0.238 (2)	0.5	0.070 (5)	K 0.34 (2)	3.9 (17)
M4	0.0	0.0	0.5	Mg 0.28 (3)	9.9 (19)
W1	0.309 (3)	0.0	0.097 (6)	O 0.72 (3)	3.0 (13)
W3	0.0788 (11)	0.4207 (12)	0.972 (2)	O 0.914 (14)	6.2 (13)
W4	0.5	0.0	0.5	O 1.0	5.5 (18)
W5	0.054 (3)	0.097 (3)	0.525 (8)	O 0.37 (3)	9.7 (21)
W6	0.057 (3)	0.0	0.249 (7)	O 0.74 (3)	4.5 (14)
W7	0.072 (5)	0.0	0.751 (12)	O 0.69 (3)	2.9 (11)
W8	0.071 (4)	0.0	0.035 (11)	O 0.37 (3)	2.5 (10)

C

clinoptilolite

Buckhorn, New Mexico, USA

SG C2/m

a (Å) 17.6605 (16)

b (Å) 17.9770 (17)

c (Å) 7.4056 (6)

 β (°) 116.343 (7)V (Å³) 2107.0 (3)

Site	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>B</i> _{iso}
T1	0.1777	0.1687	0.0926	Si 1.0	1.58
T2	0.2129	0.4113	0.4997	Si 1.0	1.82
T3	0.2107	0.1905	0.7141	Si 1.0	1.73
T4	0.0696	0.298	0.4182	Si 1.0	1.58
T5	0.0	0.2203	0.0	Si 1.0	2.29
O1	0.2021	0.5	0.461	O 1.0	0.79
O2	0.2324	0.1225	0.61	O 1.0	2.61
O3	0.1836	0.1553	0.878	O 1.0	3.95
O4	0.2375	0.1135	0.26	O 1.0	4.66
O5	0.0	0.3225	0.5	O 1.0	4.26
O6	0.0803	0.1667	0.057	O 1.0	1.34
O7	0.126	0.2325	0.56	O 1.0	2.29
O8	0.0097	0.2708	0.189	O 1.0	1.73
O9	0.2141	0.2486	0.183	O 1.0	3.87
O10	0.1203	0.3719	0.414	O 1.0	3.32
M1	0.150 (2)	0.0	0.643 (5)	Na 0.258 (4) Ca 0.135	4.5 (11)
M2	0.028 (2)	0.5	0.177 (3)	Ca 0.423 (8)	6.7 (8)
M3	0.247 (2)	0.5	0.072 (6)	K 0.36 (2)	9.2 (13)
M4	0.0	0.0	0.5	Mg 0.32 (3)	10.0 (11)
W1	0.309 (3)	0.0	0.053 (5)	O 0.64 (2)	3.0 (12)
W3	0.0723 (10)	0.4172 (9)	0.974 (3)	O 0.875 (11)	6.5 (7)
W4	0.5	0.0	0.5	O 1.0	7.9 (11)
W5	0.034 (2)	0.094 (2)	0.434 (6)	O 0.39 (3)	13.4 (14)
W6	0.051 (3)	0.0	0.280 (6)	O 0.60 (2)	2.8 (14)
W7	0.093 (5)	0.0	0.742 (9)	O 0.59 (4)	13.5 (12)
W8	0.068 (3)	0.0	0.054 (8)	O 0.53 (3)	6.1 (9)

E

mordenite

Mangatarem, Luzon,
PhilippinesSG Cmc_m

a (Å) 18.0860 (19)

b (Å) 20.4543 (17)

c (Å) 7.5210 (6)

V (Å³) 2787.8 (8)

Site	<i>x</i>	<i>y</i>	<i>z</i>	Occupancy	<i>B</i> _{iso}
T1	0.19808	0.42723	0.54187	Si 1.0	1.8
T2	0.19673	0.19088	0.54521	Si 1.0	1.8
T3	0.08692	0.38266	0.25	Si 1.0	1.8
T4	0.08621	0.22661	0.25	Si 1.0	1.8
O1	0.1234	0.4154	0.4285	O 1.0	2.2
O2	0.1232	0.194	0.4254	O 1.0	2.2
O3	0.2621	0.3773	0.4868	O 1.0	2.2
O4	0.0965	0.305	0.25	O 1.0	2.2
O5	0.1692	0.1948	0.75	O 1.0	2.2
O6	0.1768	0.4202	0.75	O 1.0	2.2
O7	0.2296	0.5	0.5	O 1.0	2.2
O8	0.25	0.25	0.5	O 1.0	2.2
O9	0.0	0.406	0.25	O 1.0	2.2
O10	0.0	0.205	0.25	O 1.0	2.2
M1	0.0	0.5	0.0	Ca 0.24 (2)	1.8
M2	0.0	0.998 (2)	0.75	Ca 0.42 (3)	1.8
W1	0.0	0.448 (4)	0.75	O 1.0	3.1 (8)
W2	0.0	0.270 (2)	0.75	O 1.0	5.0 (7)
W3	0.0	0.161 (2)	0.75	O 0.85 (3)	8.8 (12)
W4	0.021 (4)	0.071 (4)	0.035 (2)	O 0.52 (2)	12.3 (14)
W5	0.125 (3)	0.021 (3)	0.75	O 0.85 (4)	13.4 (15)

G

mordenite

Cabo de Gata, Almeria, Spain

SG Cmc_m

a (Å) 18.1033 (13)

b (Å) 20.4481 (13)

c (Å) 7.5167 (4)

V (Å³) 2787.8 (8)

Site	<i>x</i>	<i>y</i>	<i>z</i>		Occupancy	Biso
T1	0.19808	0.42723	0.54187	Si	1.0	1.8
T2	0.19673	0.19088	0.54521	Si	1.0	1.8
T3	0.08692	0.38266	0.25	Si	1.0	1.8
T4	0.08621	0.22661	0.25	Si	1.0	1.8
O1	0.1234	0.4154	0.4285	O	1.0	2.2
O2	0.1232	0.194	0.4254	O	1.0	2.2
O3	0.2621	0.3773	0.4868	O	1.0	2.2
O4	0.0965	0.305	0.25	O	1.0	2.2
O5	0.1692	0.1948	0.75	O	1.0	2.2
O6	0.1768	0.4202	0.75	O	1.0	2.2
O7	0.2296	0.5	0.5	O	1.0	2.2
O8	0.25	0.25	0.5	O	1.0	2.2
O9	0.0	0.406	0.25	O	1.0	2.2
O10	0.0	0.205	0.25	O	1.0	2.2
M1	0.0	0.5	0.0	Ca	0.44 (2)	1.8
M2	0.0	0.991 (3)	0.75	Ca	0.35 (2)	1.8
W1	0.0	0.442 (4)	0.75	O	1.0	7.1
W2	0.0	0.275 (2)	0.75	O	0.78 (3)	1.3
W3	0.0	0.150 (3)	0.75	O	0.63 (3)	5.0
W4	0.019 (3)	0.069 (5)	0.034 (2)	O	0.561 (17)	17.8
W5	0.116 (3)	0.041 (6)	0.75	O	0.96 (3)	17.2

References

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