

Supporting Information

Zeolite structure determination using genetic algorithms and geometry optimisation.

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Table S1. Volume and cell parameters variation of 28 candidate zeolites using different force fields. “X” means that the zeolite structure optimisation did not result in a tetracoordinated structure.

Zeolite Codename	initial structure	force-fields				
		BS	SC	SLC	VLC	
0303_64567						
a (Å)	7.5570	X	7.4854	X	7.6709	
b (Å)	18.7150	X	17.8007	X	17.9677	
c (Å)	14.0990	X	19.0933	X	19.2879	
alpha (°)	90.00	X	90.01	X	90.00	
beta (°)	90.00	X	90.10	X	90.00	
gamma (°)	90.00	X	89.97	X	90.00	
volume (Å³)	1994.0	X	2544.1	X	2658.4	
Δ(volume) (%)	0	X	28	X	33	
0310_48918						
a (Å)	7.5570	X	X	X	7.6403	
b (Å)	18.7150	X	X	X	19.0205	
c (Å)	14.0990	X	X	X	14.2577	
alpha (°)	90.00	X	X	X	91.83	
beta (°)	90.00	X	X	X	89.12	
gamma (°)	90.00	X	X	X	89.98	
volume (Å³)	1994.0	X	X	X	2070.7	
Δ(volume) (%)	0	X	X	X	4	
0902_181848						
a (Å)	7.5570	X	7.5826	X	7.7493	
b (Å)	18.7150	X	18.3071	X	18.2274	
c (Å)	14.0990	X	15.7399	X	16.4844	
alpha (°)	90.00	X	89.99	X	90.00	
beta (°)	90.00	X	89.96	X	90.00	
gamma (°)	90.00	X	90.00	X	90.00	
volume (Å³)	1994.0	X	2184.9	X	2328.4	
Δ(volume) (%)	0	X	10	X	17	
0_30894						
a (Å)	10.4500	X	10.1194	X	9.4465	
b (Å)	15.0280	X	17.3524	X	17.9595	
c (Å)	8.9540	X	9.1517	X	9.4278	
alpha (°)	90.00	X	88.56	X	90.00	
beta (°)	105.64	X	117.97	X	119.43	
gamma (°)	90.00	X	91.79	X	90.00	
volume (Å³)	1354.1	X	1418.5	X	1393.1	
Δ(volume) (%)	0	X	5	X	3	
0_34894						
a (Å)	10.4500	8.9346	9.0071	8.9508	9.3649	
b (Å)	15.0280	17.0734	17.3802	17.3409	18.1461	
c (Å)	8.9540	8.7871	8.8416	8.7548	9.0565	
alpha (°)	90.00	90.00	89.72	89.80	90.01	
beta (°)	105.64	114.01	113.44	112.36	111.25	
gamma (°)	90.00	90.00	91.37	90.70	89.94	
volume (Å³)	1354.1	1224.4	1269.5	1256.6	1434.4	
Δ(volume) (%)	0	-10	-6	-7	6	
0_44627						
a (Å)	10.4500	9.4695	9.6215	9.6979	9.8933	
b (Å)	15.0280	14.6496	14.7273	14.0507	15.1503	
c (Å)	8.9540	8.9319	9.1857	9.1794	9.2571	
alpha (°)	90.00	90.01	90.01	90.00	90.00	
beta (°)	105.64	105.57	105.58	105.52	105.67	
gamma (°)	90.00	89.91	90.03	90.00	90.00	
volume (Å³)	1354.1	1193.6	1253.8	1205.2	1335.9	
Δ(volume) (%)	0	-12	-7	-11	-1	

Zeolite Codename	initial structure	force-fields				
		BS	SC	SLC	VLC	
1_11481						
a (Å)	15.7940	15.3530	15.6817	15.5230	15.7703	
b (Å)	9.2060	8.8776	9.0527	8.9672	9.0858	
c (Å)	8.5890	8.8681	8.7940	8.7016	9.0101	
alpha (°)	90.00	90.00	90.00	90.00	90.00	
beta (°)	90.00	90.00	90.00	90.00	90.00	
gamma (°)	90.00	90.00	90.00	90.00	90.00	
volume (Å³)	1248.8	1208.7	1248.4	1211.2	1291.0	
Δ(volume) (%)	0	-3	-0	-3	3	
3_1365021						
a (Å)	18.3775	18.9275	19.2027	19.0003	19.5611	
b (Å)	18.3775	18.9275	19.2059	19.0004	19.5611	
c (Å)	18.3775	18.9275	19.2072	19.0004	19.5611	
alpha (°)	90.00	90.00	89.95	90.00	90.00	
beta (°)	90.00	90.00	89.98	90.00	90.00	
gamma (°)	90.00	90.00	90.00	90.00	90.00	
volume (Å³)	6206.7	6780.8	7083.7	6859.4	7484.8	
Δ(volume) (%)	0	9	14	11	21	
3_27767						
a (Å)	10.4500	10.0862	10.5341	10.3139	10.3981	
b (Å)	15.0280	15.5229	14.9002	15.5194	16.2471	
c (Å)	8.9540	10.0718	10.5681	10.2882	10.4983	
alpha (°)	90.00	89.95	90.10	90.00	90.00	
beta (°)	105.64	123.29	122.54	123.95	123.84	
gamma (°)	90.00	90.01	89.94	90.00	90.00	
volume (Å³)	1354.1	1318.1	1398.4	1366.1	1473.1	
Δ(volume) (%)	0	-3	3	1	9	
3_31105						
a (Å)	9.7620	X	9.4300	9.4195	9.7403	
b (Å)	20.5300	X	19.2243	19.1188	20.5447	
c (Å)	9.9960	X	9.7269	9.5348	10.1715	
alpha (°)	90.00	X	89.66	90.04	89.99	
beta (°)	96.90	X	111.70	111.88	111.36	
gamma (°)	90.00	X	91.09	90.29	89.38	
volume (Å³)	1988.8	X	1638.1	1593.4	1895.5	
Δ(volume) (%)	0	X	-18	-20	-5	
4_15364						
a (Å)	10.4500	9.0349	9.0471	8.9342	9.3667	
b (Å)	15.0280	17.1204	17.2191	16.9414	18.1544	
c (Å)	8.9540	8.9479	8.8263	8.7249	9.0531	
alpha (°)	90.00	89.74	90.54	89.37	89.99	
beta (°)	105.64	111.68	113.36	113.69	111.19	
gamma (°)	90.00	91.55	87.29	93.35	90.07	
volume (Å³)	1354.1	1285.7	1260.8	1207.1	1435.4	
Δ(volume) (%)	0	-5	-7	-11	6	
4_76033						
a (Å)	10.4500	9.7045	X	9.5623	10.0906	
b (Å)	15.0280	12.6140	X	12.6250	13.1345	
c (Å)	8.9540	10.2378	X	10.4483	10.6707	
alpha (°)	90.00	88.81	X	90.22	89.98	
beta (°)	105.64	91.46	X	90.64	90.00	
gamma (°)	90.00	89.34	X	90.26	89.97	
volume (Å³)	1354.1	1252.5	X	1261.3	1414.2	
Δ(volume) (%)	0	-8	X	-7	4	

Zeolite Codename	initial structure	force-fields				
		BS	SC	SLC	VLC	
4_98439						
a (Å)	20.7530	21.8816	20.1276	19.9907	20.7967	
b (Å)	9.8040	10.0717	8.5377	8.4790	8.7888	
c (Å)	20.0090	21.3482	21.1683	21.0387	22.0440	
alpha (°)	90.00	89.98	90.07	89.99	90.00	
beta (°)	90.00	90.00	89.95	89.99	90.00	
gamma (°)	90.00	89.99	89.71	89.92	90.00	
volume (Å³)	4071.1	4704.8	3637.6	3566.1	4029.2	
Δ(volume) (%)	0	16	-11	-12	-1	
5_27095						
a (Å)	10.4500	10.7393	X	10.2734	10.3981	
b (Å)	15.0280	16.3865	X	15.5260	16.2469	
c (Å)	8.9540	10.3624	X	10.0535	10.4984	
alpha (°)	90.00	89.96	X	90.46	89.99	
beta (°)	105.64	112.83	X	122.99	123.84	
gamma (°)	90.00	90.51	X	90.06	90.00	
volume (Å³)	1354.1	1680.6	X	1345.0	1473.1	
Δ(volume) (%)	0	24	X	-1	9	
5_51886						
a (Å)	10.4500	X	9.9155	9.4188	9.6802	
b (Å)	15.0280	X	18.3748	18.1666	18.9219	
c (Å)	8.9540	X	8.2246	8.1342	8.5263	
alpha (°)	90.00	X	90.09	89.99	90.00	
beta (°)	105.64	X	97.47	96.18	96.53	
gamma (°)	90.00	X	90.11	89.06	89.99	
volume (Å³)	1354.1	X	1485.8	1383.7	1551.6	
Δ(volume) (%)	0	X	10	2	15	
6_18831						
a (Å)	13.8830	X	14.8234	14.6896	15.0940	
b (Å)	13.8830	X	14.8234	14.6896	15.0940	
c (Å)	13.8830	X	14.8234	14.6896	15.0940	
alpha (°)	90.00	X	90.00	90.00	90.00	
beta (°)	90.00	X	90.00	90.00	90.00	
gamma (°)	90.00	X	90.00	90.00	90.00	
volume (Å³)	2675.8	X	3257.2	3169.8	3438.8	
Δ(volume) (%)	0	X	22	18	29	
6_45037						
a (Å)	10.4500	X	11.1917	11.4624	11.6346	
b (Å)	15.0280	X	16.2544	15.9760	16.8936	
c (Å)	8.9540	X	8.4678	8.5450	8.7692	
alpha (°)	90.00	X	90.13	89.89	90.00	
beta (°)	105.64	X	129.90	127.21	131.36	
gamma (°)	90.00	X	90.16	90.59	90.00	
volume (Å³)	1354.1	X	1181.7	1246.2	1293.7	
Δ(volume) (%)	0	X	-13	-8	-4	
7_31194						
a (Å)	10.4500	X	8.2911	7.9399	9.5710	
b (Å)	15.0280	X	17.7104	17.7403	17.5714	
c (Å)	8.9540	X	8.1488	8.0694	8.5686	
alpha (°)	90.00	X	90.21	90.05	89.36	
beta (°)	105.64	X	119.56	120.68	121.46	
gamma (°)	90.00	X	89.88	89.97	90.39	
volume (Å³)	1354.1	X	1040.8	977.5	1229.1	
Δ(volume) (%)	0	X	-23	-28	-9	

Zeolite Codename	initial structure	force-fields			
		BS	SC	SLC	VLC
7_5188					
a (Å)	10.4500	X	9.3250	X	9.9819
b (Å)	15.0280	X	15.0865	X	16.0973
c (Å)	8.9540	X	9.3258	X	9.5120
alpha (°)	90.00	X	90.01	X	90.00
beta (°)	105.64	X	109.33	X	108.52
gamma (°)	90.00	X	89.99	X	90.00
volume (Å³)	1354.1	X	1238.0	X	1449.3
Δ(volume) (%)	0	X	-9	X	7
8_111416					
a (Å)	14.1040	X	13.3542	12.7772	12.0032
b (Å)	18.2050	X	18.0420	18.8631	19.8944
c (Å)	7.4770	X	7.3133	7.4351	8.0238
alpha (°)	90.00	X	89.37	90.34	89.78
beta (°)	98.99	X	102.62	101.72	97.49
gamma (°)	90.00	X	88.64	90.79	90.10
volume (Å³)	1896.2	X	1718.7	1754.4	1899.7
Δ(volume) (%)	0	X	-9	-7	0
8_33283					
a (Å)	10.4500	12.8077	12.9054	12.7180	13.1290
b (Å)	15.0280	13.3500	13.8170	13.6790	14.0876
c (Å)	8.9540	7.8992	7.7366	7.6331	8.0702
alpha (°)	90.00	90.05	90.00	89.94	90.00
beta (°)	105.64	112.48	111.43	111.22	112.35
gamma (°)	90.00	89.86	90.00	89.89	90.00
volume (Å³)	1354.1	1248.0	1284.2	1237.9	1380.5
Δ(volume) (%)	0	-8	-5	-9	2
8_46824					
a (Å)	10.4500	12.4406	12.7266	12.4578	X
b (Å)	15.0280	13.4591	13.6363	13.5365	X
c (Å)	8.9540	9.1620	9.2483	9.1983	X
alpha (°)	90.00	90.02	90.12	90.00	X
beta (°)	105.64	83.37	84.10	82.97	X
gamma (°)	90.00	90.02	90.04	90.00	X
volume (Å³)	1354.1	1523.8	1596.5	1539.5	X
Δ(volume) (%)	0	13	18	14	X
9_13403					
a (Å)	15.7940	14.9435	16.0031	15.7307	16.5490
b (Å)	9.2060	10.2807	9.7416	9.6914	9.8910
c (Å)	8.5890	9.9469	9.0215	8.6831	8.8905
alpha (°)	90.00	90.01	90.00	90.04	90.00
beta (°)	90.00	90.00	90.00	90.15	90.00
gamma (°)	90.00	89.97	90.00	90.02	90.00
volume (Å³)	1248.8	1528.1	1406.4	1323.8	1455.3
Δ(volume) (%)	0	22	13	6	17
9_25035					
a (Å)	10.4500	X	9.5953	9.3969	9.6570
b (Å)	15.0280	X	18.3705	18.1149	18.9108
c (Å)	8.9540	X	8.2279	8.1393	8.5132
alpha (°)	90.00	X	90.00	89.99	90.00
beta (°)	105.64	X	96.71	96.07	96.54
gamma (°)	90.00	X	90.00	89.99	90.00
volume (Å³)	1354.1	X	1440.4	1377.7	1544.6
Δ(volume) (%)	0	X	6	2	14

Zeolite Codename	initial structure	force-fields				
		BS	SC	SLC	VLC	
9_28607						
a (Å)	10.4500	X	X	10.1646	11.0901	
b (Å)	15.0280	X	X	14.2739	13.2663	
c (Å)	8.9540	X	X	8.6155	8.6572	
alpha (°)	90.00	X	X	89.40	90.25	
beta (°)	105.64	X	X	100.83	104.74	
gamma (°)	90.00	X	X	89.53	90.55	
volume (Å³)	1354.1	X	X	1227.6	1231.7	
Δ(volume) (%)	0	X	X	-9	-9	
9_3540						
a (Å)	10.4500	X	X	10.4039	9.6658	
b (Å)	15.0280	X	X	18.2517	19.5466	
c (Å)	8.9540	X	X	7.4603	7.9514	
alpha (°)	90.00	X	X	91.04	89.93	
beta (°)	105.64	X	X	92.00	89.95	
gamma (°)	90.00	X	X	92.04	90.01	
volume (Å³)	1354.1	X	X	1414.6	1502.3	
Δ(volume) (%)	0	X	X	4	11	
9_3746						
a (Å)	10.4500	X	X	X	11.6801	
b (Å)	15.0280	X	X	X	13.5592	
c (Å)	8.9540	X	X	X	8.0315	
alpha (°)	90.00	X	X	X	90.06	
beta (°)	105.64	X	X	X	101.16	
gamma (°)	90.00	X	X	X	90.00	
volume (Å³)	1354.1	X	X	X	1247.9	
Δ(volume) (%)	0	X	X	X	-8	
9_42398						
a (Å)	10.4500	12.3991	12.5037	12.2969	12.7420	
b (Å)	15.0280	11.9741	12.4813	12.4605	12.7543	
c (Å)	8.9540	8.6404	8.8993	8.7053	9.0175	
alpha (°)	90.00	91.97	90.06	89.38	90.02	
beta (°)	105.64	89.66	91.10	90.01	90.05	
gamma (°)	90.00	90.30	89.88	90.02	89.97	
volume (Å³)	1354.1	1282.0	1388.6	1333.8	1465.5	
Δ(volume) (%)	0	-5	3	-1	8	