Supplementary Material (ESI) for Chemical Communications

Supplementary information

Table S1. Cell parameters and atomic coordinates of the optimised cell AST zeolite framework type of composition $[DABCOH,F]_2$-$Si_{20}O_{40}$, where DABCOH is protonated 1,4-diazabicyclo [2.2.2] octane. The forcefield in [14] was used for the optimisation. C2 is secondary carbon, N3 is tertiary nitrogen and N4 is cuaternary nitrogen. O2 is oxygen in Si-O-Si bridges.

CELL PARAMETERS

8.977609	8.972038	13.504335	89.888547	90.215739	90.271662

ATOM	X	Y	Z
Si1	0.22763	0.05076	0.10271
Si1	0.75732	0.95269	0.10387
Si1	0.94572	0.23414	0.10445
Si1	0.04035	0.76964	0.10313
Si1	0.75820	0.95511	0.88011
Si1	0.22953	0.05208	0.87913
Si1	0.04108	0.77047	0.88005
Si1	0.94743	0.23600	0.87938
Si1	0.72912	0.54718	0.60326
Si1	0.25787	0.45208	0.60432
Si1	0.44781	0.73433	0.60427
Si1	0.54045	0.26583	0.60291
Si1	0.25879	0.45820	0.38023
Si1	0.72822	0.55019	0.37918
Si1	0.53882	0.27237	0.37930
Si1	0.44874	0.73673	0.38023
Si2	0.49308	0.00403	0.24185
Si2	0.99390	0.50239	0.24099
Si2	0.49314	0.00112	0.74127
Si2	0.99465	0.50315	0.74266
C2	0.04695	0.95110	0.56104
N3	0.08092	0.09007	0.50262
C2	0.93839	0.16527	0.47237
C2	0.84705	0.05826	0.40726
N4	0.92775	0.91206	0.39524
C2	0.95349	0.84490	0.49664
C2	0.16830	0.04952	0.41189
C2	0.07625	0.94289	0.34733
H	0.86503	0.83982	0.35084
H	0.15160	0.89843	0.58455
H	0.98731	0.98056	0.62910
H	0.87567	0.19774	0.53855
H	0.96486	0.26891	0.43248
H	0.73799	0.03716	0.44119
H	0.82690	0.10942	0.33434
H	0.00837	0.73602	0.49036
H	0.84590	0.82505	0.53265
H	0.19490	0.14960	0.36872
H	0.27415	0.99937	0.43513
H	0.13837	0.83987	0.33312
H	0.05569	0.99539	0.27532
C2	0.61341	0.58923	0.11963
N3	0.61867	0.65428	0.01694
C2	0.46303	0.68958	0.98273
C2	0.36832	0.54648	0.98483

N4	0.46337	0.41503	0.01520
C2	0.52471	0.44260	0.11811
C2	0.68838	0.54410	0.94730
C2	0.59238	0.40200	0.94418
H	0.40023	0.31694	0.01434
H	0.72726	0.57080	0.14617
H	0.56353	0.66947	0.17084
H	0.41535	0.77588	0.03056
H	0.46706	0.73735	0.90780
H	0.27584	0.55898	0.03716
H	0.31729	0.52791	0.91173
H	0.59750	0.35044	0.14119
H	0.43359	0.44719	0.17211
H	0.69910	0.59320	0.87300
H	0.80214	0.51879	0.97241
H	0.65988	0.30488	0.96442
H	0.55171	0.38236	0.86848
F	0.99870	0.00029	0.99402
F	0.49841	0.50155	0.48511
O2	0.36943	0.08260	0.17356
O2	0.61584	0.92346	0.17474
O2	0.91413	0.37913	0.17219
O2	0.07274	0.62625	0.17251
O2	0.61515	0.92211	0.81119
O2	0.37251	0.08204	0.81038
O2	0.07267	0.62744	0.81139
O2	0.91432	0.38309	0.81391
O2	0.87192	0.58083	0.67238
O2	0.11705	0.42359	0.67493
O2	0.41486	0.87574	0.67375
O2	0.57264	0.12296	0.67149
O2	0.11501	0.42430	0.31169
O2	0.86983	0.58167	0.30874
O2	0.57067	0.12934	0.31010
O2	0.41544	0.88129	0.31225
O2	0.29400	0.06367	0.99172
O2	0.69565	0.95669	0.99193
O2	0.92498	0.29531	0.99218
O2	0.06208	0.70543	0.99190
O2	0.79324	0.56636	0.49103
O2	0.19612	0.44395	0.49154
O2	0.43517	0.79915	0.49203
O2	0.55550	0.20492	0.49011
O2	0.17216	0.88455	0.13528
O2	0.81858	0.11694	0.13837
O2	0.11388	0.18241	0.13298
O2	0.87389	0.82218	0.13257
O2	0.81889	0.11924	0.84746
O2	0.17148	0.88635	0.84959
O2	0.87261	0.82196	0.85428
O2	0.11570	0.18572	0.85350
O2	0.67488	0.37987	0.63007
O2	0.31623	0.61895	0.63115
O2	0.61433	0.67798	0.63191
O2	0.37713	0.32506	0.63230
O2	0.31434	0.62464	0.34943
O2	0.67407	0.38328	0.34829
O2	0.37392	0.32841	0.34742
O2	0.61415	0.68202	0.34774

Table S2. Cell parameters and atomic coordinates of the optimised cell AST zeolite framework type of composition $[DABCOH,F]_2$-$Si_{19}Ge_1O_{40}$, where DABCOH is protonated 1,4-diazabicyclo [2.2.2] octane. The forcefield in [14] was used for the optimisation. C2 is secondary carbon, N3 is tertiary nitrogen and N4 is cuaternary nitrogen. O2 and O3 are oxygens in Si-O-Si and Si-O-Ge bridges respectively

---

CELL PARAMETERS

8.828761	9.005639	13.590707	89.875825	91.319808	90.787176

ATOM	X	Y	Z
Si1	0.22763	0.05076	0.10271
Si1	0.75410	0.94676	0.10416
Si1	0.94183	0.23080	0.09966
Si1	0.04207	0.76679	0.10287
Si1	0.74755	0.94437	0.88186
Si1	0.22006	0.04770	0.88116
Si1	0.03542	0.76112	0.88040
Si1	0.93451	0.23055	0.87582
Ge1	0.70662	0.54675	0.59471
Si1	0.25082	0.44398	0.60606
Si1	0.43681	0.73742	0.60795
Si1	0.54414	0.25735	0.61016
Si1	0.25465	0.44821	0.38086
Si1	0.73972	0.55302	0.37790
Si1	0.54662	0.26414	0.38380
Si1	0.44624	0.73561	0.38087
Si2	0.49441	0.00058	0.24393
Si2	0.99371	0.49838	0.23457
Si2	0.47890	0.99366	0.74388
Si2	0.98178	0.49958	0.73966
C2	0.09953	0.09414	0.62334
N3	0.10638	0.15251	0.51968
C2	0.94785	0.17832	0.48091
C2	0.85585	0.03271	0.48749
N4	0.95750	0.90776	0.52109
C2	0.01953	0.94196	0.62335
C2	0.18362	0.04114	0.45594
C2	0.08812	0.89737	0.45183
H	0.89708	0.80750	0.52180
H	0.21443	0.08668	0.65476
H	0.03949	0.17218	0.66989
H	0.89558	0.26606	0.52408
H	0.95190	0.21902	0.40470
H	0.76420	0.04422	0.54013
H	0.80147	0.00784	0.41576
H	0.10012	0.85649	0.64763
H	0.92779	0.94116	0.67669
H	0.19945	0.08609	0.38158
H	0.29745	0.01935	0.48673
H	0.15751	0.80175	0.47268
H	0.04580	0.87713	0.37635
C2	0.60451	0.58406	0.11516
N3	0.60642	0.64698	0.01256
C2	0.44693	0.67923	0.97818
C2	0.35162	0.53540	0.98166
N4	0.45023	0.40661	0.01249
C2	0.51573	0.43638	0.11453
C2	0.67622	0.53709	0.94424
C2	0.57888	0.39443	0.94170

H	0.38662	0.30814	0.01235
H	0.72127	0.56788	0.14145
H	0.55473	0.66376	0.16576
H	0.39907	0.76554	0.02475
H	0.44844	0.72486	0.90316
H	0.25997	0.54679	0.03426
H	0.29665	0.51500	0.90945
H	0.59133	0.34604	0.13761
H	0.42489	0.44005	0.16836
H	0.68540	0.58508	0.87012
H	0.79244	0.51339	0.96989
H	0.64805	0.29839	0.96207
H	0.53471	0.37391	0.86666
F	0.99594	0.99775	0.99311
F	0.53664	0.50738	0.51143
O2	0.37280	0.08469	0.17463
O2	0.61488	0.91755	0.17736
O2	0.91074	0.37736	0.16453
O2	0.07921	0.62142	0.16932
O2	0.59815	0.90877	0.81463
O2	0.36100	0.08164	0.81020
O2	0.06672	0.61721	0.81439
O2	0.90204	0.37392	0.80824
O3	0.86637	0.58422	0.67252
O2	0.10791	0.41609	0.67475
O2	0.38571	0.87848	0.67307
O2	0.56515	0.10699	0.67251
O2	0.11152	0.41605	0.30846
O2	0.86705	0.58115	0.29655
O2	0.57639	0.12223	0.31509
O2	0.41183	0.87935	0.31327
O2	0.29213	0.06368	0.99186
O2	0.68780	0.94555	0.99294
O2	0.91698	0.29045	0.98770
O2	0.05945	0.70198	0.99248
O3	0.81458	0.56861	0.48405
O2	0.19785	0.44802	0.49158
O2	0.42158	0.79079	0.49246
O2	0.56640	0.20501	0.49552
O2	0.17601	0.88338	0.13380
O2	0.81387	0.11351	0.13402
O2	0.11430	0.18391	0.12875
O2	0.87369	0.81774	0.13173
O2	0.80459	0.10898	0.84671
O2	0.16542	0.88063	0.85015
O2	0.86434	0.81473	0.85424
O2	0.10360	0.17708	0.84950
O3	0.67795	0.36433	0.64489
O2	0.31475	0.60898	0.63404
O3	0.60691	0.70214	0.63943
O2	0.37466	0.31816	0.63046
O2	0.32139	0.61049	0.35108
O2	0.67375	0.38519	0.35450
O2	0.37680	0.32133	0.35958
O2	0.61488	0.68184	0.35582

Table S3. Cell parameters and atomic coordinates of the optimised cell AST zeolite framework type of composition $[DABCOH,F]_2$-$Ge_{20}O_{40}$, where DABCOH is protonated 1,4-diazabicyclo [2.2.2] octane. The forcefield in [14] was used for the optimisation. C2 is secondary carbon, N3 is tertiary nitrogen and N4 is cuaternary nitrogen. O1 is oxygen in Ge-O-Ge bridges.

CELL PARAMETERS

9.314092	9.091654	14.330846	91.193881	90.431706	88.892181

ATOM	X	Y	Z
Ge1	0.22763	0.05076	0.10271
Ge1	0.74714	0.92872	0.09896
Ge1	0.92378	0.22958	0.10058
Ge1	0.05323	0.75183	0.10022
Ge1	0.75563	0.93509	0.87480
Ge1	0.22992	0.05454	0.87794
Ge1	0.05095	0.77140	0.88344
Ge1	0.93271	0.23459	0.87475
Ge1	0.72763	0.55076	0.60271
Ge1	0.24714	0.42872	0.59897
Ge1	0.42378	0.72958	0.60058
Ge1	0.55323	0.25183	0.60021
Ge1	0.25563	0.43509	0.37481
Ge1	0.72991	0.55453	0.37794
Ge1	0.55095	0.27139	0.38343
Ge1	0.43270	0.73459	0.37475
Ge2	0.49314	0.00461	0.24197
Ge2	0.98939	0.49555	0.24142
Ge2	0.48939	0.99555	0.74142
Ge2	0.99314	0.50462	0.74198
C2	0.03670	0.93767	0.55601
N3	0.08233	0.07775	0.51204
C2	0.95243	0.16561	0.48097
C2	0.86570	0.07366	0.41027
N4	0.93993	0.92698	0.39232
C2	0.95094	0.84793	0.48387
C2	0.17505	0.04175	0.42894
C2	0.08884	0.95308	0.35639
H	0.88205	0.86465	0.34337
H	0.13114	0.87498	0.58045
H	0.97192	0.96372	0.61815
H	0.88723	0.19899	0.54163
H	0.98721	0.26751	0.44887
H	0.75844	0.05345	0.43767
H	0.85081	0.13398	0.34508
H	0.99909	0.73749	0.47376
H	0.84256	0.83428	0.51104
H	0.21118	0.14338	0.39798
H	0.27258	0.98269	0.45149
H	0.14322	0.84772	0.33976
H	0.08123	0.01444	0.29133
C2	0.53669	0.43778	0.05605
N3	0.58233	0.57781	0.01202
C2	0.45243	0.66565	0.98093
C2	0.36569	0.57363	0.91027
N4	0.43993	0.42695	0.89236
C2	0.45096	0.34796	0.98393
C2	0.67505	0.54174	0.92894
C2	0.58883	0.45303	0.85641

Supplementary Material (ESI) for Chemical Communications

H	0.38205	0.36459	0.84343
H	0.63113	0.37511	0.08053
H	0.47190	0.46389	0.11816
H	0.38724	0.69909	0.04157
H	0.48722	0.76751	0.94878
H	0.25845	0.55344	0.93769
H	0.35078	0.63390	0.84506
H	0.49914	0.23753	0.97385
H	0.34258	0.33429	0.01110
H	0.71121	0.64333	0.89794
H	0.77257	0.48268	0.95151
H	0.64321	0.34767	0.83980
H	0.58121	0.51436	0.79134
F	0.99990	0.96410	0.96904
F	0.49988	0.46411	0.46904
O1	0.37207	0.09651	0.17071
O1	0.60376	0.89996	0.16883
O1	0.88867	0.38196	0.17042
O1	0.08883	0.60795	0.17332
O1	0.60500	0.89441	0.80940
O1	0.38054	0.09729	0.81592
O1	0.09302	0.61548	0.81098
O1	0.89356	0.38824	0.81082
O1	0.87207	0.59652	0.67071
O1	0.10376	0.39997	0.66883
O1	0.38867	0.88196	0.67042
O1	0.58883	0.10795	0.67331
O1	0.10499	0.39442	0.30941
O1	0.88053	0.59729	0.31592
O1	0.59301	0.11547	0.31097
O1	0.39355	0.88823	0.31082
O1	0.27504	0.10117	0.99193
O1	0.70201	0.88943	0.98524
O1	0.94351	0.29352	0.98941
O1	0.05437	0.67981	0.98884
O1	0.77503	0.60117	0.49193
O1	0.20201	0.38942	0.48525
O1	0.44351	0.79352	0.48941
O1	0.55436	0.17982	0.48884
O1	0.19916	0.86582	0.11427
O1	0.77999	0.11726	0.10691
O1	0.07975	0.14869	0.14261
O1	0.89354	0.82941	0.13899
O1	0.78867	0.11927	0.85958
O1	0.20443	0.86926	0.85858
O1	0.88472	0.81250	0.83368
O1	0.09370	0.16471	0.83481
O1	0.69916	0.36582	0.61427
O1	0.27999	0.61726	0.60691
O1	0.57975	0.64868	0.64261
O1	0.39354	0.32942	0.63899
O1	0.28865	0.61927	0.35958
O1	0.70442	0.36925	0.35858
O1	0.38471	0.31250	0.33368
O1	0.59369	0.66471	0.33481