Supporting Information

Synthesis and characterization of a layer aluminosilicate NUD-11 and its transformation to a 3D stable zeolite

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Table S1 Crystallographic data for NUD-11

Compound reference	NUD-11
Empirical formula	$C_{45}H_{59}FN_{10}O_{40}Si_{18}$
Formula weight	1904.64
Temperature/K	293
Crystal system	Monoclinic
Space group	*C 2/c*
a/Å	15.767(4)
b/Å	26.561(6)
c/Å	7.380(2)
β/°	91.264(6)
Unit cell volume/ /Å^3	3090(1)
Z	2
No. of reflections collected	9208
No. of independent reflections	3339
R_{int}	0.1391
Final R_1 values ($I > 2\sigma(I)$)[a]	0.0923
Final $wR(F^2)$ values ($I > 2\sigma(I)$)[a]	0.2111
Final R_1 values (all data)[a]	0.1889
Final $wR(F^2)$ values (all data)[a]	0.2606
Goodness of fit on F^2	1.018
largest diff. peak and hole (e Å^{-3})	0.944 and -0.821
CCDC	2011086

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2. Atomic coordinates, thermal parameters (Å) and occupancies for NUD-11S structure model (Triclinic *P1*, *a* = 15.7670 Å, *b* = 22.850 Å, *c* = 7.380 Å, *β* = 91.264°)

Atoms	*x*	*y*	*z*	U_{ani}	Occ.
Si1	0.72408	0.62090	0.07765	0.01771	1
Si2	0.57408	0.70881	0.11192	0.01229	1
Si3	0.71008	0.80320	0.23860	0.01281	1
Si4	0.67061	0.80237	0.64944	0.01360	1
O5	0.72108	0.55005	0.14685	0.01735	1
O6	0.63072	0.65047	0.08067	0.01944	1
O7	0.63597	0.76473	0.14229	0.02344	1
O8	0.73466	0.86102	0.10801	0.02260	1
O9	0.67660	0.81946	0.43649	0.02050	1
O10	0.70891	0.73968	0.70864	0.02267	1
O11	0.71995	0.85206	0.75654	0.02282	1
O12	0.57396	0.80349	0.70670	0.01822	1
O13	0.46058	0.72682	0.59896	0.01693	1
Si14	0.22383	0.12095	0.07772	0.01771	1

Si15	0.07401	0.20898	0.11196	0.01229	1
Si16	0.21013	0.30324	0.23866	0.01281	1
Si17	0.17058	0.30245	0.64946	0.01360	1
O18	0.22056	0.05011	0.14666	0.01735	1
O19	0.13054	0.15062	0.08062	0.01944	1
O20	0.13598	0.26485	0.14222	0.02344	1
O21	0.23478	0.36104	0.10810	0.02260	1
O22	0.17661	0.31953	0.43651	0.02050	1
O23	0.20882	0.23974	0.70866	0.02267	1
O24	0.21996	0.35212	0.75656	0.02282	1
O25	0.07391	0.30363	0.70671	0.01822	1
O26	0.96044	0.22699	0.59910	0.01693	1
Si27	0.27782	0.62006	0.47508	0.01771	1
Si28	0.42922	0.70768	0.39970	0.01229	1
Si29	0.29134	0.79175	0.23346	0.01281	1
Si30	0.31864	0.8183	0.82435	0.01360	1
O31	0.28244	0.55244	0.57165	0.01735	1
O32	0.37054	0.64888	0.42941	0.01944	1
O33	0.37850	0.76039	0.29781	0.02344	1
O34	0.27023	0.84290	0.37064	0.02260	1
O35	0.29573	0.82206	0.03538	0.02050	1
O36	0.28209	0.75805	0.74954	0.02267	1
O37	0.27986	0.87238	0.69896	0.02282	1
O38	0.41915	0.81231	0.81111	0.01822	1
O39	0.51542	0.72393	0.93502	0.01693	1
Si40	0.77800	0.12012	0.47516	0.01771	1
Si41	0.92922	0.20783	0.39978	0.01229	1
Si42	0.79126	0.29181	0.23352	0.01281	1
Si43	0.81851	0.31843	0.82458	0.0136	1
O44	0.78278	0.05252	0.57166	0.01735	1
O45	0.87066	0.14898	0.42934	0.01944	1
O46	0.87844	0.26046	0.29769	0.02344	1
O47	0.77018	0.34287	0.37099	0.02260	1
O48	0.79567	0.32223	0.03563	0.02050	1
O49	0.78202	0.25812	0.74999	0.02267	1
O50	0.77959	0.37245	0.69913	0.02282	1
O51	0.91903	0.31250	0.81114	0.01822	1
O52	0.01527	0.22413	0.93518	0.01693	1
Si53	0.27637	0.38152	0.91118	0.01771	1
Si54	0.42620	0.29351	0.87692	0.01229	1
Si55	0.29010	0.19923	0.75022	0.01281	1
Si56	0.32965	0.20000	0.33942	0.01360	1
O57	0.27952	0.45236	0.84212	0.01735	1
O58	0.36969	0.35189	0.90825	0.01944	1

O59	0.36421	0.23765	0.84667	0.02344	1
O60	0.26544	0.14143	0.88082	0.02260	1
O61	0.32363	0.18293	0.55238	0.02050	1
O62	0.29139	0.26271	0.28017	0.02267	1
O63	0.28027	0.15031	0.23240	0.02282	1
O64	0.42631	0.19882	0.28213	0.01822	1
O65	0.53978	0.27546	0.38977	0.01693	1
Si66	0.77626	0.88155	0.91114	0.01771	1
Si67	0.92624	0.79364	0.87683	0.01229	1
Si68	0.79024	0.69924	0.75017	0.01281	1
Si69	0.82975	0.70007	0.33933	0.01360	1
O70	0.77919	0.95240	0.84190	0.01735	1
O71	0.86964	0.85199	0.90818	0.01944	1
O72	0.86432	0.73772	0.84655	0.02344	1
O73	0.76566	0.64142	0.88074	0.02260	1
O74	0.82374	0.68298	0.55228	0.02050	1
O75	0.79142	0.76275	0.28007	0.02267	1
O76	0.78048	0.65036	0.23219	0.02282	1
O77	0.92642	0.69897	0.28214	0.01822	1
O78	0.03993	0.77560	0.38970	0.01693	1
Si79	0.72223	0.38234	0.51365	0.01771	1
Si80	0.57100	0.29464	0.58908	0.01229	1
Si81	0.70896	0.21064	0.75530	0.01281	1
Si82	0.68171	0.18402	0.16423	0.01360	1
O83	0.71750	0.44995	0.41714	0.01735	1
O84	0.62956	0.35349	0.55947	0.01944	1
O85	0.62178	0.24201	0.69117	0.02344	1
O86	0.73002	0.15958	0.61780	0.02260	1
O87	0.70455	0.18021	0.95318	0.02050	1
O88	0.71821	0.24433	0.23884	0.02267	1
O89	0.72063	0.13000	0.28968	0.02282	1
O90	0.58119	0.18995	0.17768	0.01822	1
O91	0.48494	0.27834	0.05369	0.01693	1
Si92	0.22246	0.88239	0.51357	0.01771	1
Si93	0.07110	0.79479	0.58906	0.01229	1
Si94	0.20895	0.71066	0.75512	0.01281	1
Si95	0.18171	0.68405	0.16413	0.01360	1
O96	0.21794	0.95005	0.41721	0.01735	1
O97	0.12972	0.85362	0.55947	0.01944	1
O98	0.12181	0.74214	0.69123	0.02344	1
O99	0.22980	0.65956	0.61758	0.02260	1
O100	0.20462	0.68028	0.95309	0.02050	1
O101	0.21828	0.74430	0.23896	0.02267	1
O102	0.22053	0.62998	0.28952	0.02282	1

O103	0.08120	0.69007	0.17746	0.01822	1
O104	0.98497	0.77850	0.05365	0.01693	1
Si105	0.49292	0.76677	0.76463	0.01126	1
Si106	-0.00719	0.26695	0.76472	0.01126	1
Si107	0.50741	0.23551	0.22413	0.01126	1
Si108	0.00749	0.73566	0.22405	0.01126	1
O109	0.51350	0.69527	0.28306	0.01730	1
O110	0.01355	0.19548	0.28330	0.01730	1
O111	0.48666	0.30699	0.70555	0.01730	1
O112	-0.01327	0.80715	0.70550	0.01730	1
Si113	0.23293	1.50373	0.70675	0	1
Si114	0.73290	1.00329	0.70422	0	1
Si115	0.26726	0.99851	0.28089	0	1
Si116	0.76737	1.49907	0.28418	0	1
C117	0.83828	0.45600	0.13501	0	1
C118	0.84112	0.53939	0.44149	0	1
C119	0.15673	0.46412	0.55309	0	1
C120	0.16462	0.54741	0.85955	0	1
C121	0.66159	1.04624	0.85286	0	1
C122	0.65963	0.96282	0.54625	0	1
C123	1.34489	1.03767	0.43236	0	1
C124	1.33410	0.95447	0.12615	0	1

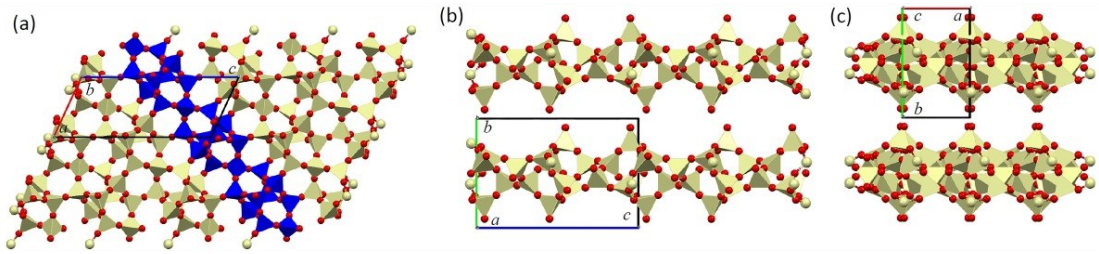

Fig. S1 Polyhedral views of RUB-39 along (a) the *b*-axis, (b) the *a*-axis, (c) the *c*-axis. The SDAs are omitted for clarity.

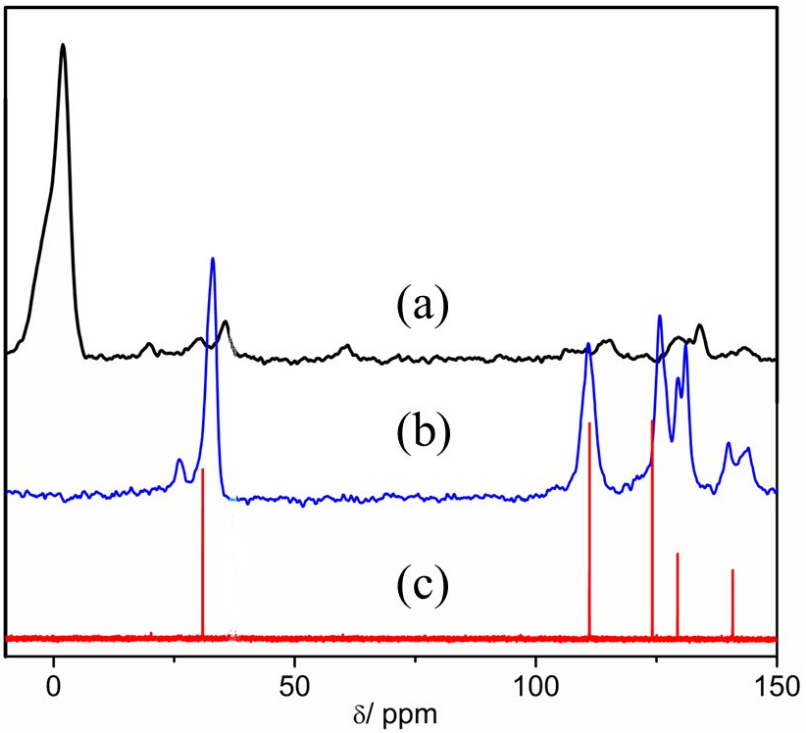

Fig. S2 ^{13}C MAS NMR spectra of (a) NUD-11S after silylated with DEDMS in 2 M HNO_3 without calcination and (b) the pristine NUD-11, and (c) ^{13}C MAS NMR spectra of DMBI iodide salt in D_2O.

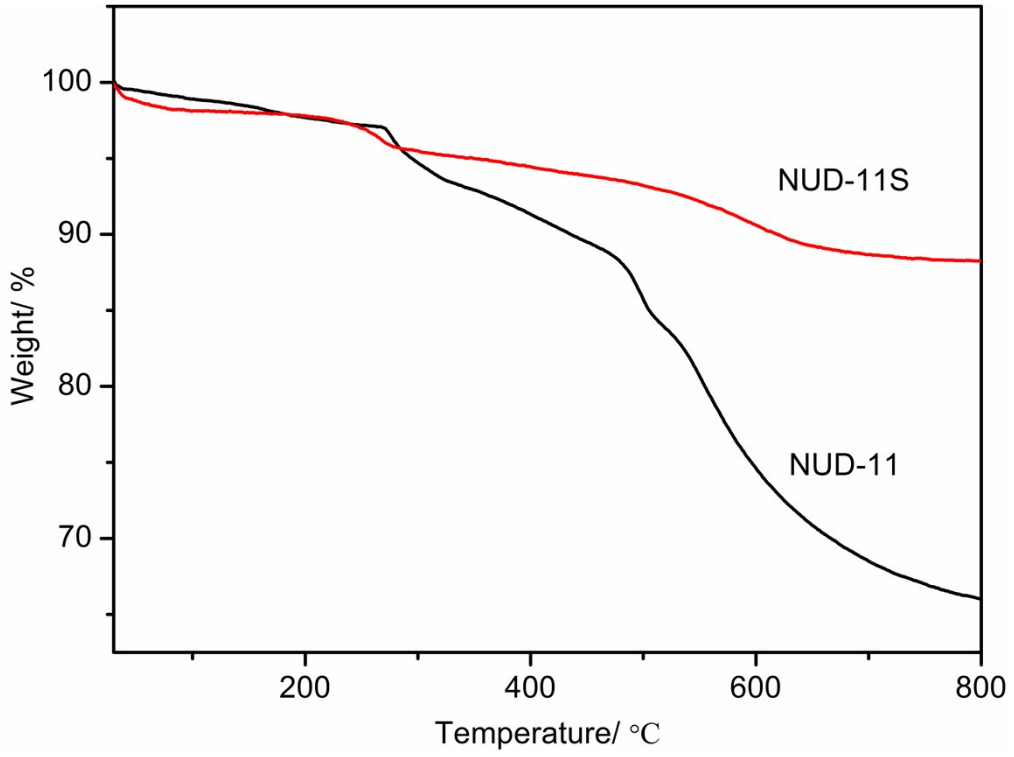

Fig. S3 Thermogravimetric analysis of NUD-11 and NUD-11S.

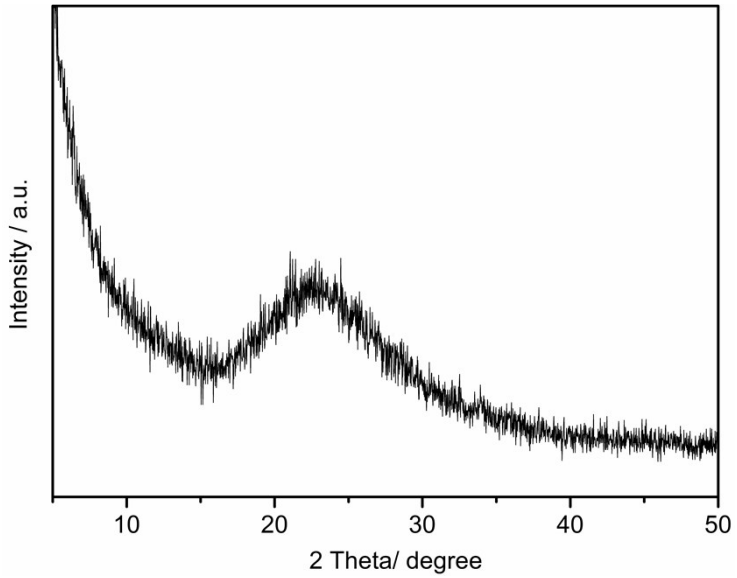

Fig. S4 PXRD pattern of NUD-11 after calcined at 550°C.

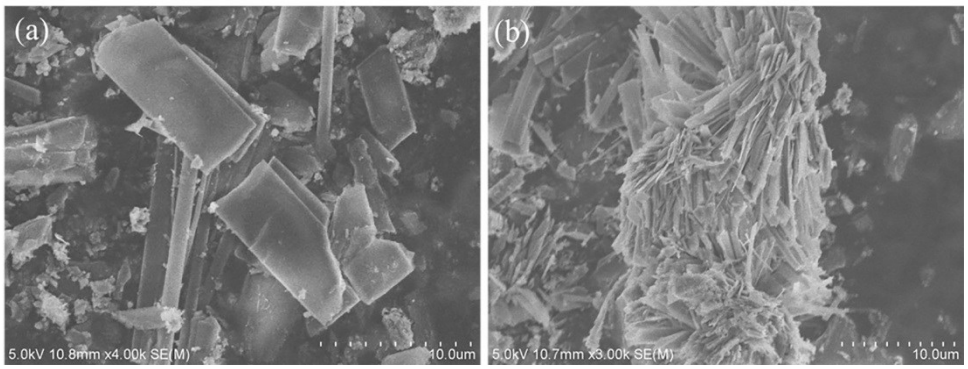

Fig. S5 SEM images of NUD-11S and NUD-11S-cal.

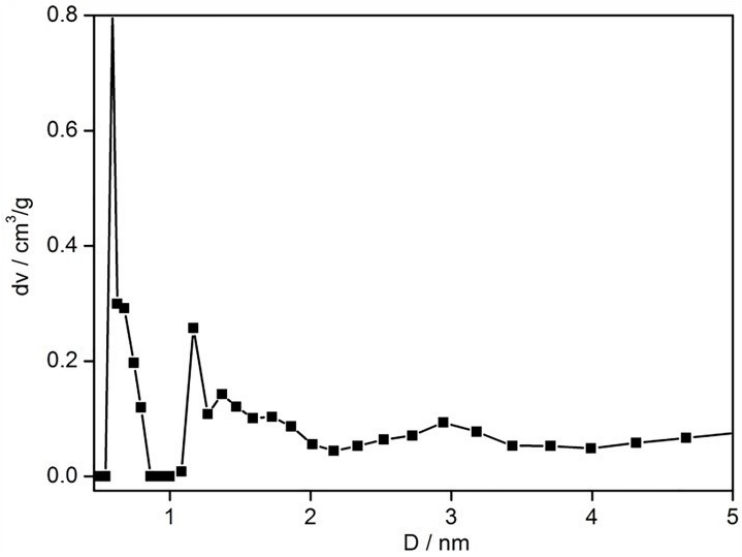

Fig. S6 DFT pore size distribution curve of NUD-11S.

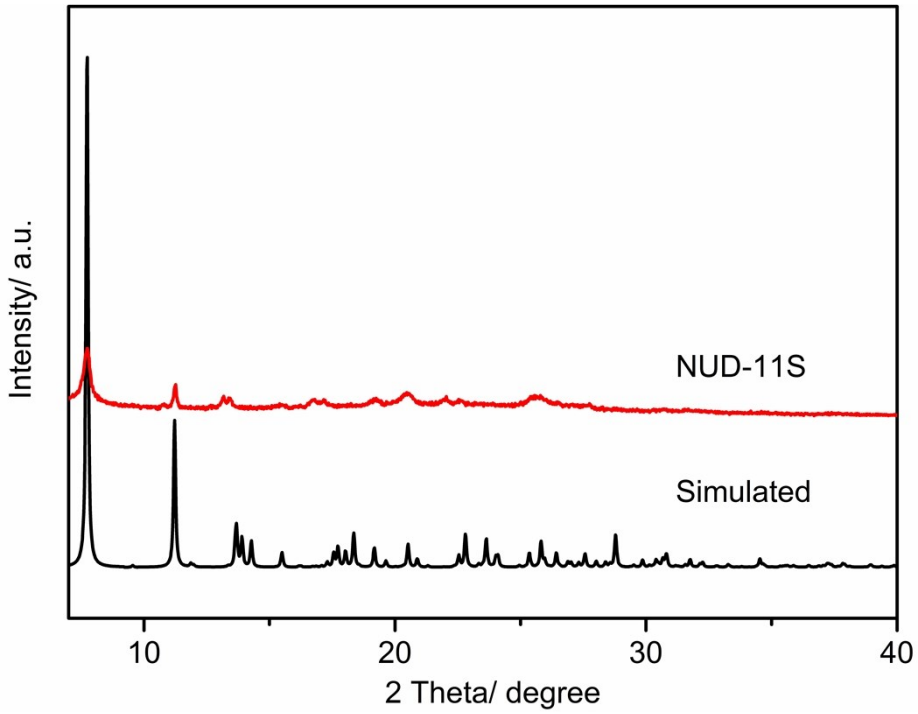

Fig. S7 PXRD patterns of NUD-11S and the simulated one based on the structure model.