Enhanced Framework Rigidity of a Zeolitic Metal-Azolate via Ligand Substitution

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1. Powder X-ray Diffraction

Data was collected in a D8 Advance Bruker AXS h–2h diffractometer, with a copper radiation source (Cu Ka, k = 1.5406 Å) and a secondary monochromator, operated at 40 kV and 30 mA. The program MERCURY 3.0 was used to obtain the diffraction patterns calculated from SCXRD data. The purity of the bulk was always verified by comparison of the calculated and observed X-ray powder diffraction patterns.

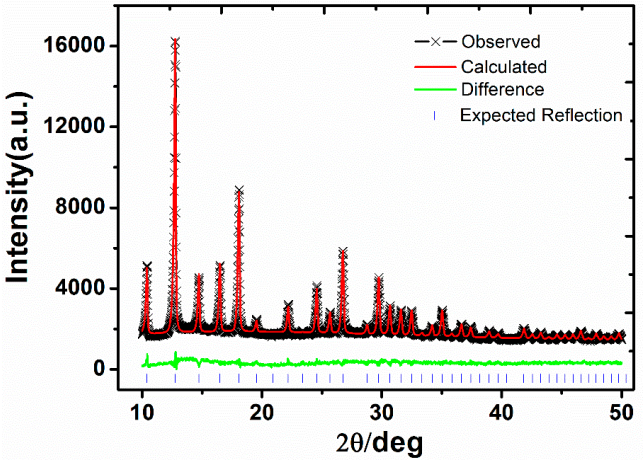

Figure S1. The powder X-ray diffraction (PXRD) spectra of MAF-7 refined by Le Bail method. The black and red symbols, and the purple continuous lines are experimental, calculated, and difference profiles, respectively, and the vertical markers indicate the allowed Bragg reflections. R_p = 5.0%, R_{wp} = 7.4% and GOF = 4.598.

Table S1. Lattice parameters and unit cell volume of MAF-7 at various pressure (GPa).

Pressure	Lattice parameter (Å)						Unit cell volume (Å³)	
GPa	a	a-errors	b	b-errors	c	c-errors	V	V-errors
0	16.9811	0.0023	16.9665	0.0025	17.0077	0.0036	4900.1	1.4
0.177	16.9058	0.0039	16.8966	0.0047	16.9164	0.007	4832.2	2.6
0.46	16.6943	0.012	16.669	0.0115	16.734	0.0179	4656.7	6.8
0.826	16.4215	0.0059	16.3821	0.0094	16.2924	0.0189	4383	5.9
1.454	16.2564	0.0091	16.1232	0.0122	16.0821	0.01692	4215.2	5.9
1.848	16.1731	0.0114	16.0466	0.0154	15.9859	0.0214	4148.7	7.4
2.244	16.1224	0.0091	15.9653	0.0176	15.9001	0.0189	4092.7	7
2.829	15.9470	0.0075	16.0272	0.0188	15.4722	0.0174	3954.5	6.7
3.313	15.9275	0.0139	15.9204	0.0266	15.5328	0.0181	3938.7	8.7
3.755	15.8421	0.009	16.0058	0.0238	15.4198	0.0159	3909.9	7.4