

Table S12 Relative Total Electronic Energies E_{rel} (in kcal/mol) of the Isomers of Zeolite Systems ZOH for Different Si/Al Ratios and Al Distributions Determined at the PBE-D3/6-31+G(d) Optimized Geometries and Corresponding Single Point E_{rel} Determined at the PBE-D3/6-31++G(2d,2p) and M06-2X-D3/6-31++G(2d,2p) Levels in Cluster Model.

Zeolite Systems ZOH	E_{rel}		
	PBE-D3/ 6-31+G(d)	PBE-D3/ 6-31++G(2d,2p)	M06-2X-D3/ 6-31++G(2d,2p)
(31Si,1Al)			
Al1	0.0	0.0	0.0
Al2	3.3	2.7	2.5
Al3	1.6	1.8	3.7
Al4	3.8	4.0	4.4
(30Si,2Al)			
Al1Al2	1.2	0.9	0.0
Al1Al3	0.0	0.0	1.2
Al1Al4	2.7	2.9	2.5
Al2Al3	3.7	3.3	4.1
Al2Al4	4.9	4.2	3.7
Al3Al4	3.8	3.9	5.0
(29Si,3Al)			
Al1Al2Al3	0.0	0.0	0.4
Al1Al2Al4	1.5	1.3	0.0
Al1Al3Al4	1.1	1.2	1.7
Al2Al3Al4	3.3	2.7	2.9
(28Si,4Al)			
Al1Al2Al3Al4	0.0	0.0	0.0