

Table S10 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 and PBE-D3 levels in cluster and periodic models

Cluster model (32T)			Periodic model (96T)		
Zeolite systems ZOH	E_{rel}		Zeolite systems ZOH	E_{rel}	
	PBE/ 6-31+G(d)	PBE-D3/ 6-31+G(d)		PBE	PBE-D3
(31Si,1Al)			(95Si,1Al)		
Al1	0.0	0.0	Al1	3.8	2.3
Al2	3.6	3.3	Al2	0.4	0.6
Al3	1.7	1.6	Al3	0.0	0.0
Al4	4.5	3.8	Al4	4.2	2.9
(30Si,2Al)			(94Si,2Al)		
Al1Al2	1.5	1.2	Al1Al2	4.9	3.1
Al1Al3	0.0	0.0	Al1Al3	3.7	2.8
Al1Al4	3.4	2.7	Al1Al4	8.5	6.1
Al2Al3	4.2	3.7	Al2Al3	0.0	0.0
Al2Al4	6.0	4.9	Al2Al4	3.9	2.5
Al3Al4	4.7	3.8	Al3Al4	6.1	4.5
(29Si,3Al)			(93Si,3Al)		
Al1Al2Al3	0.0	0.0	Al1Al2Al3	0.0	0.0
Al1Al2Al4	2.3	1.5	Al1Al2Al4	4.9	4.0
Al1Al3Al4	1.6	1.1	Al1Al3Al4	6.0	4.8
Al2Al3Al4	4.4	3.3	Al2Al3Al4	0.8	1.0
(28Si,4Al)			(92Si,4Al)		
Al1Al2Al3Al4	0.0	0.0	Al1Al2Al3Al4	0.0	0.0