Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Table S1. Characteristics of CO adsorption complexes formed on Brønsted-acid sites in the vicinity of each of 8 distinguishable framework Al positions; structural parameters, stretching frequencies, and energy (enthalpy) values are given in Å, cm^{-1}, and kJ mol^{-1}, respectively.

BA site	ΔE_{rel}	Al-O-Si	r(OH)	r(OH)/CO	ΔH^0(0K)	$\nu_{(OH)}$	$\nu_{(OH)}$/CO	$\Delta\nu_{(OH)}$	$\nu_{(CO)}$
$T1_{Al}$_O3H_$T4_{Si}$	**0.0**	**128.1**	**0.9755**	**1.0020**	**-24.4**	**3629**	**3280**	**349**	**2183**
$T1_{Al}$_O4H_$T7_{Si}$[a]	0.4	125.8	0.9929			3400			
$T1_{Al}$_O2H_$T6_{Si}$	4.4	127.7	0.9771	0.9966	-21	3608	3352	256	2176
$T2_{Al}$_O10H_$T8_{Si}$	**0.0**	**129.2**	**0.9756**	**0.9994**	**-24.5**	**3628**	**3314**	**314**	**2181**
$T2_{Al}$_O9H_$T5_{Si}$[a]	3.6	135.3	0.9941			3385			
$T2_{Al}$_O11H_$T3_{Si}$	6.5	136.5	0.9780			3597			
$T3_{Al}$_O13H_$T3_{Si}$	**0.0**	**132.4**	**0.9765**	**1.0022**	**-23.2**	**3617**	**3278**	**339**	**2179**
$T3_{Al}$_O12H_Si3	3.2	133.9	0.9798	1.0007	-20.3	3574	3298	276	2172
$T3_{Al}$_O11H_$T2_{Si}$	8.7	138.2	0.9787	1.0074	-23.6	3588	3210	378	2182
$T4_{Al}$_O3H_$T1_{Si}$	**0.0**	**129.0**	**0.9759**	**1.0031**	**-25.0**	**3624**	**3266**	**358**	**2183**
$T4_{Al}$_O7H_$T4_{Si}$	2.6	140.0	0.9784	1.0026	-22.4	3591	3273	319	2181
$T4_{Al}$_O6H_$T5_{Si}$	8.3	142.6	0.9793			3579			
$T5_{Al}$_O8H_$T5_{Si}$[a]	**0.0**	**138.4**	**0.9919**	**0.9994**	**-17.1**	**3414**	**3315**	**100**	**2178**
$T5_{Al}$_O9H_$T2_{Si}$	1.6	138.5	0.9794			3578			
$T5_{Al}$_O6H_$T4_{Si}$	5.1	142.3	0.9796	1.0008	-19.8	3576	3296	280	2177
$T6_{Al}$_O2H_$T1_{Si}$	**0.0**	**127.7**	**0.9761**	**0.9968**	**-19.6**	**3621**	**3349**	**272**	**2177**
$T6_{Al}$_O1H_$T6_{Si}$	34.6	148.3	0.9856			3497			
$T7_{Al}$_O4H_$T1_{Si}$[a]	**0.0**	**128.2**	**0.9919**	**0.9923**	**0.1**	**3413**	**3408**	**5**	**2139**
$T7_{Al}$_O5H_$T8_{Si}$[a]	38.7	147.7	1.0045			3247			
$T8_{Al}$_O10H_$T2_{Si}$	**0.0**	**131.6**	**0.9753**	**0.9985**	**-25.0**	**3633**	**3326**	**306**	**2180**
$T8_{Al}$_O5H_$T7_{Si}$[a]	25.4	149.4	1.0137			3127			

[a] Brønsted-acid sites involved in intra-zeolite hydrogen bonding.