Table S9. Totally and partially optimized intermolecular geometrical parameters of PYH^+/ZO^- adsorption complexes with one to four Al atoms calculated at the PBE-D3 level in periodic model

PYH^+/ZO^- Adsorption complexes	Total optimization			Partial optimization		
	O…H[a]	N–H[a]	O…H–N[b]	O…H[a]	N–H[a]	O…H–N[b]
1 Al						
$Al1_{ads}$	1.707	1.060	170.8	1.731	1.059	173.6
$Al2_{ads}$	1.622	1.070	174.2	1.601	1.072	173.8
$Al3_{ads}$	1.624	1.067	170.8	1.581	1.071	174.8
$Al4_{ads}$	1.769	1.054	153.7	1.763	1.051	147.3
2Al						
$Al1_{ads}Al2$	1.711	1.064	173.2	1.716	1.063	172.3
$Al1_{ads}Al3$	1.695	1.064	170.1	1.698	1.064	171.9
$Al1_{ads}Al4$	1.679	1.064	173.3	1.715	1.062	176.4
$Al2_{ads}Al1$	1.626	1.074	170.8	1.607	1.074	171.1
$Al2_{ads}Al3$	1.627	1.072	173.4	1.610	1.075	173.6
$Al2_{ads}Al4$	1.651	1.068	174.3	1.637	1.069	173.9
$Al3_{ads}Al1$	1.599	1.073	173.3	1.566	1.075	174.8
$Al3_{ads}Al2$	1.650	1.066	164.6	1.621	1.070	168.6
$Al3_{ads}Al4$	1.615	1.069	170.6	1.618	1.068	171.1
$Al4_{ads}Al1$	1.759	1.054	154.6	1.770	1.051	147.9
$Al4_{ads}Al2$	1.728	1.061	155.7	1.719	1.057	149.8
$Al4_{ads}Al3$	1.730	1.057	154.0	1.734	1.055	149.0
3 Al						
$Al1_{ads}Al2Al3$	1.677	1.069	175.0	1.659	1.072	176.0
$Al1_{ads}Al2Al4$	1.692	1.065	175.6	1.670	1.067	171.6
$Al1_{ads}Al3Al4$	1.689	1.068	173.2	1.708	1.065	174.1
$Al2_{ads}Al1Al3$	1.627	1.075	169.7	1.647	1.072	166.9
$Al2_{ads}Al1Al4$	1.612	1.075	170.7	1.617	1.074	171.3
$Al2_{ads}Al3Al4$	1.643	1.069	172.2	1.635	1.071	172.5
$Al3_{ads}Al1Al2$	1.696	1.065	172.5	1.613	1.072	170.2
$Al3_{ads}Al1Al4$	1.607	1.071	171.9	1.589	1.073	173.3
$Al3_{ads}Al2Al4$	1.648	1.067	168.9	1.574	1.074	170.9
$Al4_{ads}Al1Al2$	1.713	1.061	156.6	1.722	1.057	149.7
$Al4_{ads}Al1Al3$	1.742	1.056	153.0	1.730	1.055	149.3
$Al4_{ads}Al2Al3$	1.720	1.061	154.8	1.699	1.060	150.5
4 Al						
$Al1_{ads}Al2Al3Al4$	1.667	1.070	173.6	1.652	1.072	175.0
$Al2_{ads}Al1Al3Al4$	1.619	1.075	169.6	1.607	1.079	169.5
$Al3_{ads}Al1Al2Al4$	1.605	1.074	167.3	1.652	1.085	169.7
$Al4_{ads}Al1Al2Al3$	1.675	1.066	162.4	1.688	1.061	150.9

[a]In Å; [b]In deg.