Supporting Information

Table S1 The bond parameters (Å) calculated in solution phase for the studied compounds

Compound	V−O_d	V−O_c	V−O_t	C−O_c	V−X
a3	1.813	2.021	1.610	1.279	2.547
a4	1.814	2.023	1.613	1.281	2.906
a5	1.813	2.025	1.613	1.282	3.051
b1	1.807	2.003	1.603	1.286	
b2	1.810	2.008	1.612	1.282	[a]2.746
b3	1.813	2.020	1.614	1.280	2.532
b4	1.813	2.022	1.616	1.282	2.903
b5	1.812	2.024	1.616	1.282	3.049

[a]The distance between V atom and O_1 atom in NO_3 unit.