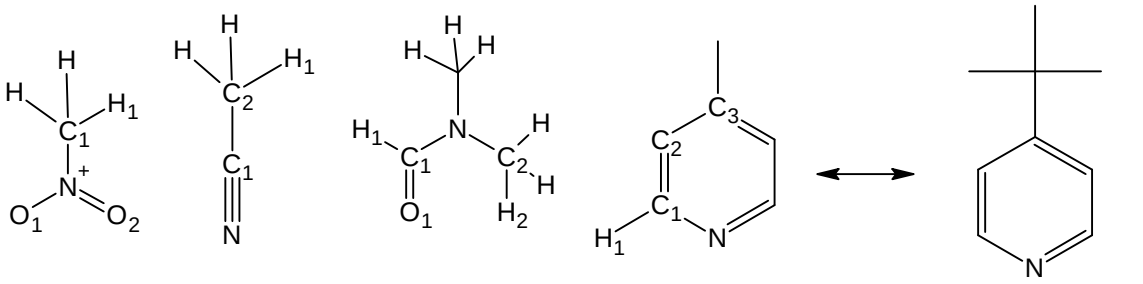
Supporting Information

Table S1. Main Structural parameters (distance in Å and angles in degrees) computed for the adsorbate molecules adsorbed on ZnO or in the gas phase (vac). For labeling scheme refer to Figure SI.1

	MP/ZnO	**MP/vac**		**MeCN/ZnO**	**MeCN/vac**
d(N-C_1)	1.342	1.335	d(C_1-C_2)	1.444	1.456
d(C_1-C_2)	1.387	1.389	d(C_2-N)	1.157	1.157
d(C_3-C_4)	1.505	1.505	d(C_1-H_1)	1.115	1.095
d(N-Zn_1)	2.113	-	d(H_1-O_1)	2.007	-
d(H_1-O_1)	2.061	-	d(N-Zn_1)	2.165	-
d(H_2-O_2)	2.283	-	a(C_1-C_2-N)	176.34	180
d(C_1-H_1)	1.098	1.092			
	NM/ZnO	**NM/vac**		**DMF/ZnO**	**DMF/vac**
d(C-N)	1.478	1.492	d(C_1-O_3)	1.236	1.213
d(C-H_1)	1.095	1.090	d(C_1-N)	1.331	1.359
d(C-H_2)	1.095	1.090	d(C_2-N)	1.460	1.447
d(N-O_1)	1.224	1.218	d(C_2-H_1)	1.099	1.092
d(N-O_2)	1.223	1.218	d(C_2-H_2)	1.101	1 .099
d(O_1-Zn_1)	2.277	-	d(O_3-Zn_1)	2.074	-
d(O_2-Zn_2)	2.284	-	d(H_1-O_1)	2.146	-
d(H_1-O_3)	2.230	-	d(H_2-O_2)	2.203	-
d(H_2-O_4)	2.227	-	a(O_3-C_1-N)	124.74	125.61
a(O_1-N-O_2)	123.45	125.70			

Figure S1. Structure and labeling scheme for NM, MeCN, DMF, MP and TBP (from left to right).



Nitromethane NM | Acetonitrile MeCN | Diméthylformamide DMF | p-méthylpyridine MP | p-tertbutylpyridine TBP

Figure S2. Basic representation of a hexagonal cell and of its plane (100) together with the directions [100], [001] and [120] and the *a* and *b* parameters.