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Electronic supplementary information for:

Ammonia-modified Co(II) sites in zeolites: IR spectroscopy and spin-resolved charge transfer analysis for NO adsorption complexes

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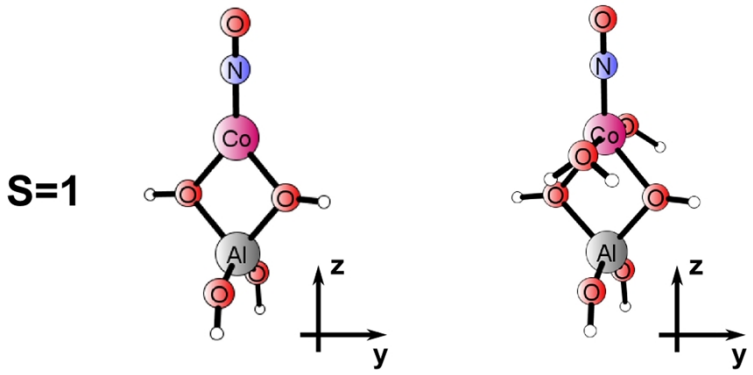

Fig. S1. Optimized geometry of $[T1Co(NO)]^+$ (left) and $[T1Co(H_2O)_2(NO)]^+$ (right)

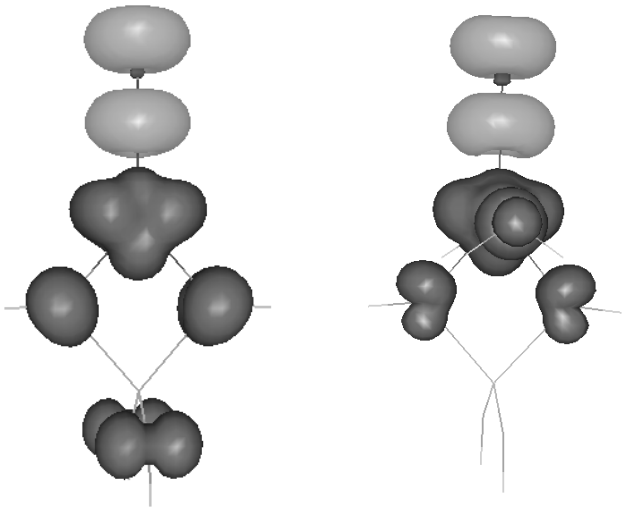

Fig. S2. Spin densities for triplet complexes $[T1Co(NO)]^+$ (left) and $[T1Co(H_2O)_2(NO)]^+$ (right)

Table S1. The comparison of calculated charge and spin densities of $[T1Co(NO)]^+$ and $[T1Co(H_2O)_2(NO)]^+$ models

Model	Q^{NO} a)				$\rho_S{}^{NO}$ a)			
	NO	**Co**	**O** b)	**O** c)	**NO**	**Co**	**O** b)	**O** c)
$[T1Co(NO)]^+$	0.21	0.70	-0.54	——	0.40	2.00	0.11	——
$[T1Co(H_2O)_2(NO)]^+$	0.22	0.55	-0.55	-0.51	0.43	2.19	0.04	0.07

a) from Mulliken population analysis
b) oxygen atom from Co-O-Al unit
c) oxygen atom from water molecule

Table S2. Geometric parameters calculated for studied systems *(available experimental values for pentaaminenitrosylcobalt(II) complex [g] in italics)*

Model	$[T1Co(NO)]^+$	$[T1Co(H_2O)_2(NO)]^+$	$[T1Co(NH_3)_3(NO)]^+$		$[Co(NH_3)_5(NO)]^{2+}$
	——	**(a)**	**(b_S)**	**(b_T)**	**(c)**
$\alpha_{Co\text{-}N\text{-}O}$ /deg	180	180	122	148	123 (*119*)
$\alpha_{Al\text{-}Co\text{-}N}$ /deg	180	180	129	142	———
$d_{Co\text{-}NO}$ /Å	1.67	1.69	1.79	1.70	1.84 (*1.87*)
$d_{N\text{-}O}$ /Å	1.14	1.14	1.19	1.16	1.17 (*1.15*)
$d_{Co\text{-}NH_3}$ /Å	———	———	2[a]	2.15[a]	2.03[c] (*1.98*)
			2[b]	2.19[b]	2.40[d] (*2.22*)
$d_{Co\text{-}O(H_2O)}$ /Å	———	2.19	———	———	———
			———	———	
$d_{Co\text{-}O}$ /Å [e]	1.88	1.97	1.94	2.03	———
			2.20	2.12	
$d_{Al\text{-}O}$ /Å [e]	1.88	1.86	1.82	1.81	———
			1.85	1.84	
$d_{Al\text{-}O}$ /Å [f]	1.70	1.71	1.72	1.72	———

a) in plane of Co-O-Al-O motif
b) out of plane of Co-O-Al-O motif
c) average equatorial C-NH3 bond
d) axial C-NH3 bond
e) oxygen atom from Co-O-Al unit
f) peripheral oxygen atom
g) after C.S. Pratt, B.A. Coyle, .J.A. Ibers, J. Chem. Soc. (A), 1971, 2146.

Table S3. Comparison of relative energy calculated by various exchange-correlation functionals for singlet ($\mathbf{b_S}$) and triplet ($\mathbf{b_T}$) of $[T1Co(NH_3)_3(NO)]^+$

Functional	**Relative energy (kcal/mol)**	
	(b_S)	**(b_T)**
BP86	0	5.2
PBE	0	5.0
B3LYP	3.3	0
PBE0	7.0	0
TPSSh	0	1.9