Supporting Information

Co-adsorption of aniline and H_2 over Pd/Al_2O_3: An infrared spectroscopic study

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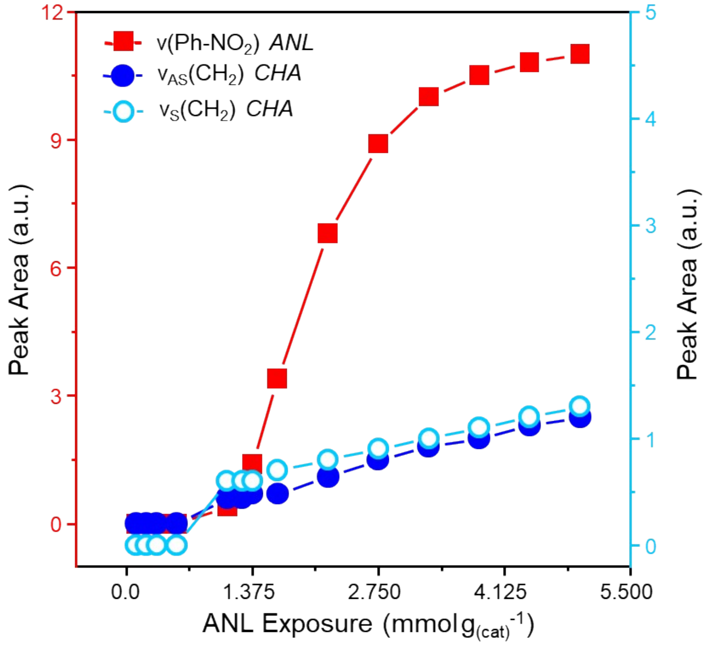
Table S1. Comparison of experimental and DFT-derived wavenumbers (cm^{-1}) of aniline.

Figure S1 *Plot of peak area for bands corresponding to a). aniline v(Ph-NH_2) mode (red squares), b) cyclohexylamine $v_S(CH_2)$ (turquoise circles), and c) $v_{AS}(CH_2)$ modes (blue circles) as a function of increasing aniline and H_2 exposure to 5wt% Pd/Al_2O_3.*

Table S1. *Comparison of experimental and DFT-derived wavenumbers (cm^{-1}) of aniline. DFT calculations performed utilising the B3LYP method and 6-311 G++(3df.2p) basis set. Vibrational assignments are based on DFT. Reproduced with from Philosophical Transactions of the Royal Society A* **2026**. https://doi.org/DOI:%252010.1098/rsta.2024.0556

Mode	Sym.	Expt.[a]	DFT	Assignment	Phenyl Contribution	
1	A'	234	220	δ_{oop}(Ph-NH_2) [f]	M20	*oop*
2	A''	277[c]	295	τ(NH_2) [f]		*ip*
3	A''	390	384	δ_{ip}(Ph-NH_2) [f]	M30	*ip*
4	A''	415	418	Ring deformation	M14	*oop*
5	A'	501	503	Ring deformation [f]	M19	*oop*
6	A'	526	535	Ring deformation[f]	M11	*ip*
7	A'	531	569	δ_{ip}(ring) + δ_{ip}(NH_2)	NH_2 wag	*ip*
8	A''	621	634	Ring deformation	M29	*ip*
9	A'	690	698	Ring deformation	M18	*oop*
10	A'	751	763	δ_{oop}(CH)	M17	*oop*
11	A'	814	825	NH_2 wag + δ_{oop}(CH)	M10	*oop*
12	A"	828	830	δ_{oop}(CH)	M13	*oop*
13	A'	880	890	δ_{oop}(CH)	M16	*oop*
14	A"	957	975	δ_{oop}(CH)	M12	oop
15	A'	968	984	δ_{oop}(ring)	M9	*ip*
16	A'	997	992	δ_{oop}(CH)	M15	*oop*
17	A'	1028	1048	δ_{ip}(ring)	M8	*ip*
18	A''	1051	1062	δ_{ip}(ring) + δ_{ip}(NH_2)	NH_2 rock + M28[e]	*ip*
19	A''	1118	1134	δ_{ip}(ring) + δ_{ip}(NH_2)	NH_2 rock + M28[e]	*ip*
20	A''	1153	1180	δ_{ip}(CH)	M27	*ip*
21	A'	1176	1202	δ_{ip}(CH)	M7	*ip*
****22**	A'	1278	1293	ν(Ph-NH_2)	M6	*ip*
23	A''	1310	1344	ν(CC)+ δ_{ip}(NH_2)	M25	*ip*
24	A''	1340 [b]	1370	δ_{ip}(CH)	M26	*ip*
****25**	A''	1498	1501	ν(CC)	M24	*ip*
26	A'	1584	1532	ν(CC)	M5	*ip*
27	A''	1590 [b]	1624	ν(CC)	M23	*ip*
****28**	A'	1601	1643	ν(CC) + δ_{ip}(NH_2)	NH_2 scissors + M4[f]	*ip*
****29**	A'	1618 [d]	1659	ν(CC) + δ_{oop}(NH_2)	NH_2 scissors + M4[f]	*oop*
30	A'	3010	3148	ν(CH)	M3	*ip*
31	A''	3025	3151	ν(CH)	M22	*ip*
32	A'	3034	3167	ν(CH)	M2	*ip*
33	A''	3054	3172	ν(CH)	M21	*ip*
34	A'	3069	3190	ν(CH)	M1	*ip*
35	A'	3353	3568	ν_s(NH_2)		*oop*
36	A''	3430	3665	ν_{as}(NH_2)		*ip*

a. Experimental wavenumbers are for aniline in the liquid phase (this work) unless otherwise indicated.
b/c/d. Reference [32]/ [33]/ [34].*The* M *number follows the assignments of* [18], *a pictorial representation is shown in Figure S1.*
e. This mode appears twice as it is mixed with the NH_2 rock.
f. This mode appears twice as it is mixed with the NH_2 scissors.



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