Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Water and Ammonia on Cu{110}: Comparative Structure and Bonding Supplementary Data

November 2, 2012

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Estimating the Zero-Point Energy Contribution to ΔH^B_{ads} Differences

We wish to estimate how much effect zero-point energy would likely have on the difference in adsorption heat between an H_2O/H_2O model for adsorption on Cu{110} and an H_2O/OH model, according to the definition of ΔH^B_{ads} where excess hydrogen H_2 desorbs from the surface.

The relevant reactions are:-

$$2H_2O(g) \rightarrow 2H_2O(a) \tag{1}$$

and

$$2H_2O(g) \rightarrow H_2O(a) + OH(a) + \frac{1}{2}H_2(g) \tag{2}$$

where (a) and (g) indicate adsorbed and gas-phase moieties.

First, we note that both adsorption models involve half of the gas-phase H_2O molecules adsorbing directly to the surface in very similar local geometries. Although zero-point energy will clearly contribute to the adsorption heat of these molecules, we can reasonably assume that this contribution will be more or less the same for both the H_2O/H_2O and the H_2O/OH models. The difference in the zero-point energy contribution to ΔH^B_{ads} between the two models must therefore derive predominantly from the adsorption of the other H_2O molecules.

In the H_2O/H_2O model, these other H_2O molecules adsorb without forming a direct bond to the surface itself. Instead, they are attached to the chemisorbed H_2O molecules via hydrogen bonds, and may be said to occupy a semi-ice configuration (i.e. their environment is halfway between ice-like and gas-like environments). Recent work by Murray and Galli [*Phys. Rev. Lett.* **108**, 105502 (2012)] indicates that the change in zero-point energy in going from gas-phase to ice-like water is an increase of around 0.12–0.13 eV per molecule (depending upon the ice phase and the density functional used in the calculations). It seems not unreasonable, therefore, to suggest that the change in zero-point energy for each semi-ice H_2O molecule will be around half this value; let us say an increase of 0.065 eV per semi-ice H_2O molecule.

In the H_2O/OH model, the dissociating H_2O molecules adsorb directly to the surface as OH, and the excess hydrogen atom desorbs as half of an H_2 molecule. The zero-point energies of gas-phase H_2O and H_2 molecules may be obtained straightforwardly from experimental frequencies, and are 0.57 eV and 0.28 eV, respectively, while that of a gas-phase OH moiety may similarly be determined to be 0.23 eV. If the O–H stretch mode of adsorbed OH were unaltered from its gas-phase value, therefore, the change in zero-point energy upon partially dissociative adsorption of OH, with desorption of excess hydrogen, would be a drop of 0.20 eV per OH moiety. To this figure must be added a correction due to redshift of the O–H bond upon adsorption, and contributions from the frustrated rotations and translations of the adsorbed OH moiety. Even on a reactive surface like Pt{111}, the O–H bond redshifts by only around 250 cm^{-1} upon adsorption [Clay, Haq and Hodgson, *Phys. Rev. Lett.* **92**, 046102 (2004)], which would correspond to a decrease in zero-point energy of 0.015 eV, so on a much less reactive surface like Cu{110} it seems reasonable to estimate a decrease of no more than around 0.005 eV. For the frustrated rotations and translations, let us estimate that they average around 150 cm^{-1} (zero-point energy 0.01 eV) so with five such modes in total we might have a contribution of 0.05 eV to the zero-point energy. Putting all of these together, we estimate that the overall change in zero-point energy upon partially dissociative adsorption of OH, with desorption of excess hydrogen, would be a drop of 0.155 eV per OH moiety

From these estimates, we can expect that zero-point energy will destabilise the H_2O/H_2O model relative to the H_2O/OH model by 0.22 eV per OH moiety. Expressing ΔH^B_{ads} per gas-phase H_2O molecule (as in the main text) this becomes approximately 0.1 eV.molecule^{-1}.

Structural Models Discussed in the Text

The following tables contain cartesian coordinates for the calculated geometries discussed in the paper. Various unit cells have been used, with lateral dimensions given below:-

(3×2) – $\mathbf{a}_1$ = (0.0000, 7.6494, 0.0000); $\mathbf{a}_2$ = (7.2120, 0.0000, 0.0000)
(2×2) – $\mathbf{a}_1$ = (0.0000, 5.0997, 0.0000); $\mathbf{a}_2$ = (7.2120, 0.0000, 0.0000)
(2×1) – $\mathbf{a}_1$ = (0.0000, 5.0997, 0.0000); $\mathbf{a}_2$ = (3.6060, 0.0000, 0.0000)

Table 1: Structure of the most stable H_2O monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 2).

Element	x	y	z
H	-1.518631	-4.248905	11.99561
H	-1.605175	-5.795324	12.03906
O	-0.967562	-5.052636	12.11474
Cu	5.409000	-1.274939	1.274914
Cu	1.803000	-1.274939	1.274914
Cu	5.409000	-3.824741	1.274914
Cu	1.803000	-3.824741	1.274914
Cu	5.409000	-6.374542	1.274914
Cu	1.803000	-6.374542	1.274914
Cu	3.606000	-5.099680	2.549827
Cu	0.000000	-5.099680	2.549827
Cu	3.606000	-2.549802	2.549827
Cu	0.000000	-2.549802	2.549827
Cu	3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	5.409000	-3.824741	3.824741
Cu	1.803000	-3.824741	3.824741
Cu	5.409000	-6.374542	3.824741
Cu	1.803000	-6.374542	3.824741
Cu	5.409000	-1.274939	3.824741
Cu	1.803000	-1.274939	3.824741
Cu	3.606000	-5.099680	5.099654
Cu	0.000000	-5.099680	5.099654
Cu	3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	3.606000	-2.549802	5.099654
Cu	0.000000	-2.549802	5.099654
Cu	5.407557	-1.273180	6.392111
Cu	1.785763	-1.276698	6.380075
Cu	5.411885	-3.829101	6.381504
Cu	1.788288	-3.831243	6.378647
Cu	5.411596	-6.373701	6.388643
Cu	1.786196	-6.373013	6.380891
Cu	3.580974	-0.006961	7.634794
Cu	-0.010457	-0.003977	7.636834
Cu	3.586023	-2.556839	7.632143
Cu	-0.010674	-2.557834	7.631327
Cu	3.589845	-5.107406	7.629899
Cu	-0.013270	-5.106947	7.679875
Cu	5.379503	-1.303701	8.977635
Cu	1.795211	-1.300565	8.958053
Cu	1.770690	-3.850367	8.964376
Cu	1.768022	-6.398408	8.969680
Cu	5.392484	-3.852585	8.957849
Cu	5.391186	-6.406670	8.966008
Cu	3.566045	-0.008797	10.09344
Cu	-0.011395	-0.042761	10.08406
Cu	3.581623	-2.567013	10.09303
Cu	-0.013198	-2.555845	10.06855
Cu	-0.009953	-5.121634	10.19319
Cu	3.561069	- 5.112761	10.07753

Table 2: Structure of the most stable OH monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 3).

Element	x	y	z
H	-1.345038	3.869719	11.73879
O	-0.378630	3.845547	11.58723
Cu	5.409000	-1.274939	1.274914
Cu	1.803000	-1.274939	1.274914
Cu	5.409000	-3.824740	1.274914
Cu	1.803000	-3.824740	1.274914
Cu	5.409000	-6.374542	1.274914
Cu	1.803000	-6.374542	1.274914
Cu	3.606000	-5.099679	2.549827
Cu	0.000000	-5.099679	2.549827
Cu	3.606000	-2.549802	2.549827
Cu	0.000000	-2.549802	2.549827
Cu	3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	5.409000	-3.824740	3.824741
Cu	1.803000	-3.824740	3.824741
Cu	5.409000	-6.374542	3.824741
Cu	1.803000	-6.374542	3.824741
Cu	5.409000	-1.274939	3.824741
Cu	1.803000	-1.274939	3.824741
Cu	3.606000	-5.099679	5.099654
Cu	0.000000	-5.099679	5.099654
Cu	3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	3.606000	-2.549802	5.099654
Cu	0.000000	-2.549802	5.099654
Cu	5.417510	-1.275857	6.398434
Cu	1.789441	-1.272109	6.394150
Cu	5.432150	-3.824511	6.406797
Cu	1.779345	-3.826270	6.400270
Cu	5.420106	-6.370794	6.396598
Cu	1.786917	-6.377755	6.400474
Cu	3.610327	0.005431	7.647033
Cu	-0.024160	-0.0026008	7.657437
Cu	3.605423	-2.546130	7.644994
Cu	-0.007645	-2.545212	7.712717
Cu	3.606577	-5.100291	7.646217
Cu	-0.008366	-5.106793	7.721080
Cu	5.399408	-1.298576	9.000482
Cu	1.786773	-1.253520	8.956420
Cu	1.779777	-3.829177	8.948873
Cu	1.777397	-6.379361	8.975595
Cu	5.394576	-3.825276	8.979267
Cu	5.405034	-6.355724	9.001502
Cu	3.594244	0.003672	10.11649
Cu	-0.006924	0.001989	10.10078
Cu	3.540227	-2.549113	10.10527
Cu	0.085606	-2.470629	10.26071
Cu	0.047960	-5.169443	10.29008
Cu	3.550035	-5.096467	10.10690

Table 3: Structure of the c(2×2) 1.0 ML H_2O phase favoured in this work, calculated in a (2×2) cell (Data for Fig. 4).

Element	x	y	z
H	-4.621089	2.819650	12.67101
H	-3.020746	1.145076	12.87908
H	0.616987	3.792868	12.87703
H	0.351801	1.129981	12.57167
H	-3.230110	3.587046	12.58166
H	-2.717986	0.371510	14.21763
H	0.890826	3.011346	14.21763
H	-1.011122	0.304194	12.67386
O	-3.665932	2.723878	12.38624
O	-2.624303	0.302970	13.24992
O	0.991722	2.941939	13.25074
O	-0.053585	0.249679	12.38808
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.409216	1.279503	6.392314
Cu	-1.803433	1.279197	6.392111
Cu	-5.409937	3.815510	6.392927
Cu	-1.802784	3.815918	6.393131
Cu	-3.606721	-0.003519	7.596241
Cu	-0.001298	-0.001428	7.693542
Cu	-3.607082	2.549215	7.692726
Cu	-0.000865	2.541668	7.601953
Cu	-5.410803	3.822497	8.952545
Cu	-1.806173	3.823568	8.957237
Cu	-5.412245	1.283328	8.956829
Cu	-1.804731	1.282665	8.953361
Cu	-3.610255	0.006375	10.01225
Cu	-0.000649	0.006426	10.16993
Cu	-3.607731	2.548195	10.17136
Cu	-0.004616	2.575172	10.02225

Table 4: Structure of the (2×1) 0.5 ML H_2O phase (Data for Fig. 6).

Element	x	y	z
H	0.673961	-0.774586	12.57799
H	1.125577	0.683609	12.26120
O	0.331283	0.111580	12.34300
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.804514	1.273384	6.403942
Cu	-1.804442	3.820304	6.403942
Cu	-0.004219	-0.002448	7.711289
Cu	-0.000902	2.545798	7.630919
Cu	-1.811402	1.284246	9.016189
Cu	-1.811727	3.818570	9.014761
Cu	-0.022141	0.000153	10.18727
Cu	-0.015362	2.560791	10.09609

Table 5: Structure of the (2×1) 1.0 ML H_2O/OH phase (Data for Fig. 6).

Element	x	y	z
H	-0.450029	-0.852764	12.31750
H	-1.691755	2.553652	12.06252
H	-0.448154	0.878824	12.30812
O	-0.043597	0.009434	12.00785
O	-0.715755	2.550490	12.00744
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	2.549827	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-1.811438	1.279911	6.365184
Cu	-1.811258	3.816377	6.364572
Cu	-0.021023	-0.003468	7.647237
Cu	-0.019148	2.547175	7.690890
Cu	-1.852510	3.806688	8.893389
Cu	-1.851465	1.285521	8.891145
Cu	-0.011720	-0.002142	10.06407
Cu	-0.140129	2.560332	10.17565

Table 6: Structure of the $H_2O \rightarrow OH$ transition state (TS1), calculated at 0.167 ML in a (3×2) cell (Data for Fig. 8).

Element	x	y	z
H	-0.336584	3.291495	7.341208
H	-2.334813	2.920649	5.910499
O	-0.722931	2.650086	6.714077
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.392557	6.354501	3.875482
Cu	-1.803866	6.355418	3.868853
Cu	-5.395946	1.281288	3.815561
Cu	-1.794995	1.274557	3.849219
Cu	-5.401211	3.821834	3.815943
Cu	-1.793336	3.805081	3.899833
Cu	-3.605134	5.058372	5.010538
Cu	0.021203	5.112301	4.983254
Cu	-3.607803	-0.004360	4.979302
Cu	0.016155	-0.011398	4.977772
Cu	-3.611120	2.536950	5.052355
Cu	0.147485	2.526318	5.081551

Table 7: Structure of the OH→O transition state (TS2), calculated at 0.167 ML in a (3×2) cell (Data for Fig. 8).

Element	x	y	z
H	-2.379744	3.847460	5.591643
O	-0.742836	3.872779	6.106071
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.392124	6.349605	3.852916
Cu	-1.786557	6.381121	3.838509
Cu	-5.398254	1.309897	3.866685
Cu	-1.784537	1.272721	3.842589
Cu	-5.411957	3.822905	3.853809
Cu	-1.773503	3.825352	3.850621
Cu	-3.563593	5.070382	5.022649
Cu	0.081568	5.190632	5.132037
Cu	-3.597346	0.000076	4.977262
Cu	0.043777	0.009179	4.971143
Cu	-3.559122	2.576039	5.025072
Cu	0.054883	2.492966	5.154858

Table 8: Structure of the $H_2O \rightarrow OH$ transition state, calculated at 1.0 ML in a (2×2) cell (Data for Fig. 9).

Element	x	y	z
H	-4.678424	2.917308	7.613783
H	-3.125681	0.847308	6.225148
H	0.467193	3.787462	7.904718
H	0.173232	1.091326	7.598357
H	-3.353868	3.877420	7.486164
H	-3.133614	0.834252	8.097996
H	0.853468	3.003288	9.214182
H	-1.263975	0.267324	7.445240
O	-3.741081	2.939288	7.289318
O	-2.699307	0.150848	7.552715
O	0.856714	2.931944	8.242061
O	-0.211672	0.254524	7.246863
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.395225	3.789808	3.870893
Cu	-1.812881	3.792256	3.859291
Cu	-5.414409	1.270528	3.877012
Cu	-1.807472	1.273690	3.884406
Cu	-3.620064	-0.042174	4.961453
Cu	0.007500	0.006324	5.143128
Cu	-3.585806	2.421367	5.292166
Cu	0.000938	2.575223	4.967445

Table 9: Structure I of the NH_3 monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 11).

Element	x	y	z
H	0.919097	2.753813	12.57860
H	-0.341416	1.674930	12.61226
H	-0.648431	3.302205	12.57534
N	-0.024304	2.569155	12.23876
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	6.374542	3.824741
Cu	-1.803000	6.374542	3.824741
Cu	-5.409000	1.274939	3.824741
Cu	-1.803000	1.274939	3.824741
Cu	-3.606000	5.099680	5.099654
Cu	0.000000	5.099680	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-3.606000	2.549802	5.099654
Cu	0.000000	2.549802	5.099654
Cu	-5.421549	1.278764	6.398842
Cu	-1.793552	1.278611	6.398638
Cu	-5.419169	3.819769	6.396394
Cu	-1.795860	3.820380	6.397822
Cu	-5.418159	6.375078	6.400066
Cu	-1.797230	6.374695	6.400270
Cu	-3.608669	2.546895	7.640914
Cu	-0.004399	2.550490	7.706189
Cu	-3.609534	5.098379	7.636018
Cu	-0.003390	5.093178	7.644994
Cu	-3.609029	-0.001147	7.636426
Cu	-0.003822	0.000765	7.654377
Cu	-5.411380	6.368958	8.969884
Cu	-1.812881	6.366434	8.977839
Cu	-5.427030	1.265454	8.969068
Cu	-1.797591	1.263541	8.973147
Cu	-5.420323	3.821451	8.966008
Cu	-1.804370	3.822522	8.973147
Cu	-3.618693	5.087211	10.09487
Cu	-0.002164	5.118498	10.07855
Cu	-3.616313	0.005661	10.09079
Cu	-0.004039	-0.034040	10.10364
Cu	-3.616818	2.545824	10.08834
Cu	-0.007789	2.546512	10.20318

Table 10: Structure II of the NH_3 monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 11).

Element	x	y	z
H	0.137893	2.681296	12.84542
H	-1.190845	1.813845	12.34443
H	-1.216160	3.462767	12.27895
N	-0.620016	2.640831	12.16594
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	6.374542	3.824741
Cu	-1.803000	6.374542	3.824741
Cu	-5.409000	1.274939	3.824741
Cu	-1.803000	1.274939	3.824741
Cu	-3.606000	5.099680	5.099654
Cu	0.000000	5.099680	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-3.606000	2.549802	5.099654
Cu	0.000000	2.549802	5.099654
Cu	-5.416140	1.281671	6.398638
Cu	-1.790018	1.279682	6.399250
Cu	-5.416500	3.821681	6.395578
Cu	-1.790163	3.823899	6.395782
Cu	-5.416429	6.377908	6.401086
Cu	-1.795716	6.377832	6.401494
Cu	-3.600014	2.553473	7.640506
Cu	-0.002019	2.553626	7.708637
Cu	-3.607082	5.104499	7.636631
Cu	-0.001154	5.100062	7.641730
Cu	-3.606505	0.003672	7.641526
Cu	-0.001442	0.007573	7.646421
Cu	-5.400634	6.389841	8.972127
Cu	-1.813602	6.388924	8.988446
Cu	-5.428689	1.288632	8.980287
Cu	-1.804587	1.283659	8.976207
Cu	-5.426814	3.836674	8.973556
Cu	-1.805524	3.842411	8.967232
Cu	-3.616024	5.099756	10.09854
Cu	0.004039	5.137392	10.07121
Cu	-3.616313	0.014764	10.10935
Cu	0.001298	-0.012392	10.08671
Cu	-3.637156	2.556916	10.08712
Cu	0.001515	2.561046	10.22215

Table 11: Structure III of the NH_3 monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 11).

Element	x	y	z
H	-0.262228	3.475389	12.63062
H	-0.228548	1.821342	12.73812
H	-1.577697	2.590726	12.15431
N	-0.555685	2.609620	12.17981
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	6.374542	3.824741
Cu	-1.803000	6.374542	3.824741
Cu	-5.409000	1.274939	3.824741
Cu	-1.803000	1.274939	3.824741
Cu	-3.606000	5.099680	5.099654
Cu	0.000000	5.099680	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-3.606000	2.549802	5.099654
Cu	0.000000	2.549802	5.099654
Cu	-5.419241	1.277387	6.402514
Cu	-1.790812	1.275857	6.405166
Cu	-5.418303	3.817168	6.403330
Cu	-1.791317	3.818851	6.406185
Cu	-5.419746	6.372247	6.404146
Cu	-1.795788	6.372630	6.407002
Cu	-3.599870	2.549266	7.645401
Cu	-0.001010	2.550184	7.716797
Cu	-3.607731	5.101210	7.645810
Cu	-0.001875	5.094861	7.648053
Cu	-3.608380	-0.001224	7.645810
Cu	-0.001803	0.003825	7.653357
Cu	-5.403591	6.379209	8.984366
Cu	-1.815188	6.379515	8.995994
Cu	-5.425948	1.276698	8.986610
Cu	-1.803866	1.270885	8.983347
Cu	-5.424578	3.830554	8.986202
Cu	-1.805164	3.833232	8.980287
Cu	-3.615664	5.095549	10.11812
Cu	0.001803	5.128212	10.07896
Cu	-3.616241	0.009638	10.11955
Cu	0.002308	-0.020195	10.09446
Cu	-3.636146	2.551714	10.09752
Cu	0.012188	2.548501	10.22379

Table 12: Structure of the NH monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 12).

Element	x	y	z
H	-1.456824	3.822140	11.73369
N	-1.000377	3.812807	10.82106
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	6.374542	3.824741
Cu	-1.803000	6.374542	3.824741
Cu	-5.409000	1.274939	3.824741
Cu	-1.803000	1.274939	3.824741
Cu	-3.606000	5.099680	5.099654
Cu	0.000000	5.099680	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-3.606000	2.549802	5.099654
Cu	0.000000	2.549802	5.099654
Cu	-5.411236	1.270655	6.380891
Cu	-1.788215	1.276316	6.390275
Cu	-5.420828	3.822599	6.346826
Cu	-1.791172	3.824052	6.436172
Cu	-5.411163	6.377526	6.379463
Cu	-1.788648	6.372247	6.385787
Cu	-3.585446	2.546512	7.626431
Cu	-0.009376	2.549419	7.651113
Cu	-3.587032	5.100292	7.624187
Cu	-0.009087	5.096314	7.648461
Cu	-3.578738	-0.003595	7.638466
Cu	-0.001010	-0.001759	7.640914
Cu	-5.414121	6.367428	8.915828
Cu	-1.795427	6.382192	8.976819
Cu	-5.415851	1.264077	8.918683
Cu	-1.792110	1.251226	8.985591
Cu	-5.414409	3.817626	8.869726
Cu	-1.865600	3.815638	9.062697
Cu	-3.704299	5.118039	10.08610
Cu	0.119142	5.170132	10.20216
Cu	-3.643430	-0.004360	10.09772
Cu	0.055388	-0.005355	10.09303
Cu	-3.706391	2.522493	10.09222
Cu	0.120296	2.450894	10.20808

Table 13: Structure of the NH_2 monomer at 0.167 ML, calculated within a (3×2) cell (Data for Fig. 12).

Element	x	y	z
H	-0.855199	3.875916	12.22489
H	0.799018	3.872244	12.25529
N	-0.017309	3.870561	11.64843
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	5.099680	2.549827
Cu	0.000000	5.099680	2.549827
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	6.374542	3.824741
Cu	-1.803000	6.374542	3.824741
Cu	-5.409000	1.274939	3.824741
Cu	-1.803000	1.274939	3.824741
Cu	-3.606000	5.099680	5.099654
Cu	0.000000	5.099680	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-3.606000	2.549802	5.099654
Cu	0.000000	2.549802	5.099654
Cu	-5.424578	1.271114	6.385787
Cu	-1.790451	1.271420	6.389867
Cu	-5.426381	3.817856	6.363756
Cu	-1.788432	3.817626	6.366205
Cu	-5.420755	6.378061	6.370080
Cu	-1.793913	6.377985	6.373956
Cu	-3.609029	2.545212	7.623983
Cu	-0.005048	2.549955	7.676611
Cu	-3.608813	5.111001	7.610520
Cu	-0.004832	5.108553	7.664576
Cu	-3.607226	0.005049	7.626839
Cu	-0.004760	0.002218	7.643362
Cu	-5.430852	6.383569	8.933983
Cu	-1.789874	6.382268	8.949485
Cu	-5.435685	1.304772	8.968252
Cu	-1.787927	1.305919	8.977839
Cu	-5.418736	3.849754	8.892165
Cu	-1.807183	3.850290	8.898081
Cu	-3.620568	5.104805	10.04102
Cu	0.003750	5.156974	10.21991
Cu	-3.618477	0.004513	10.05693
Cu	0.000000	0.014458	10.07243
Cu	-3.622588	2.568543	10.05652
Cu	-0.000361	2.553320	10.23358

Table 14: Structure of the (2×1) 0.5 ML NH_3 phase (Data for Fig. 13, structure I).

Element	x	y	z
H	0.266736	-0.421639	12.93191
H	0.175468	1.232892	12.72445
H	1.509436	0.405627	12.19695
N	0.496041	0.355599	12.31240
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.803541	1.303676	6.404758
Cu	-1.804010	3.868853	6.401902
Cu	-0.002596	0.052271	7.731484
Cu	0.004976	2.616531	7.616028
Cu	-1.803541	1.365534	8.998646
Cu	-1.805272	3.939891	9.024960
Cu	-0.008438	0.134274	10.25377
Cu	-0.003498	2.668343	10.05509

Table 15: Structure of the (2×1) 1.0 ML NH_3 phase (Data for Fig. 13, structure II).

Element	x	y	z
H	1.014368	-0.338209	12.91375
H	0.178786	1.124729	12.85011
H	1.524545	0.841443	11.89688
H	-1.257737	2.900377	14.44508
H	-1.730772	2.555437	12.90335
H	-0.565926	3.661501	13.13528
N	0.687953	0.411491	12.30424
N	-0.928112	2.778241	13.48920
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.798492	1.268845	6.412714
Cu	-1.797735	3.822803	6.412101
Cu	0.005553	-0.003978	7.753310
Cu	0.015722	2.542382	7.631735
Cu	-1.795031	1.269763	9.034751
Cu	-1.796401	3.833869	9.040463
Cu	-0.012369	-0.009077	10.34169
Cu	-0.001659	2.569920	10.06549

Table 16: Structure of the (2×1) 1.0 ML NH_3 phase (Data for Fig. 13, structure III).

Element	x	y	z
H	-1.040295	-0.649900	12.53209
H	-1.486862	0.820738	11.93829
H	-0.106702	0.722723	12.85358
H	1.055512	2.816029	12.51985
H	1.923080	2.328094	13.84617
H	0.676305	3.385303	14.03588
N	-0.682508	0.229739	12.16023
N	0.987756	2.567472	13.51510
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.804334	1.261093	6.382523
Cu	-1.804010	3.819743	6.384359
Cu	-0.001911	-0.006834	7.705781
Cu	-0.010205	2.536874	7.586246
Cu	-1.809166	1.287918	8.948873
Cu	-1.808734	3.835960	8.951729
Cu	0.005012	0.009842	10.21359
Cu	0.006311	2.591389	10.01898

Table 17: Structure of the near-c(2×2) 0.5 ML NH_3 phase, calculated in a (2×2) cell (Data for Fig. 14, structure I).

Element	x	y	z
H	-4.572552	2.808635	12.52373
H	-3.183305	1.901712	12.65857
H	0.412815	-0.528273	12.69712
H	0.437264	1.115549	12.42643
H	-3.089549	3.555530	12.50680
H	-1.011194	0.307305	12.47620
N	-3.602466	2.719697	12.21530
N	-0.031228	0.236012	12.19266
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.408423	1.294190	6.370896
Cu	-1.802711	1.293782	6.371916
Cu	-5.407774	3.831829	6.366816
Cu	-1.803793	3.832033	6.367428
Cu	-3.606577	0.024478	7.580942
Cu	0.001803	0.026518	7.672328
Cu	-3.604774	2.587208	7.682731
Cu	-0.000361	2.584403	7.584614
Cu	-5.404961	3.871046	8.912155
Cu	-1.805092	3.877675	8.912360
Cu	-5.409721	1.324278	8.911544
Cu	-1.800404	1.323615	8.913176
Cu	-3.607442	0.054209	9.998586
Cu	0.007645	0.035545	10.15566
Cu	-3.600807	2.606331	10.16422
Cu	-0.000288	2.620712	9.999198

Table 18: Structure of the (2×2) 1.0 ML NH_3 bilayer phase (Data for Fig. 14, structure II).

Element	x	y	z
H	-3.557824	2.955403	14.39122
H	-1.928056	2.920062	14.49485
H	0.495969	0.472432	14.21763
H	-0.365216	0.450911	12.79340
H	-2.615792	2.995945	13.02513
H	-3.609173	1.040278	12.70997
H	-5.059578	0.652399	11.94849
H	0.366730	3.654922	12.65632
H	1.700878	3.047196	11.81508
H	-1.149160	0.595436	14.21682
H	-4.176252	-0.515320	12.72914
H	0.761227	2.072856	12.79728
N	-2.719213	2.578283	13.95163
N	-0.352667	0.140802	13.76825
N	-4.116610	0.331427	12.17043
N	0.749904	2.853817	12.14330
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.411091	1.275118	6.381299
Cu	-1.797879	1.275679	6.382523
Cu	-5.405682	3.814439	6.381707
Cu	-1.802423	3.813980	6.381707
Cu	-3.593740	-0.008465	7.692523
Cu	0.003894	-0.012953	7.596649
Cu	-3.606216	2.521983	7.594405
Cu	0.002308	2.542076	7.690687
Cu	-5.403519	3.815918	8.917459
Cu	-1.793624	3.816683	8.930106
Cu	-5.403952	1.273078	8.921131
Cu	-1.792615	1.280982	8.933983
Cu	-3.564964	-0.001581	10.19584
Cu	-0.008510	0.008006	10.01348
Cu	-3.584436	2.575478	10.00103
Cu	-0.015001	2.539118	10.20890

Table 19: Structure of the NH_3 $\rightarrow NH_2$ transition state (TS1), calculated at 0.167 ML in a (3×2) cell (Data for Fig. 16).

Element	x	y	z
H	0.749687	3.870867	7.285111
H	-0.062961	2.175589	6.573837
H	-0.909289	3.874233	7.203134
N	-0.050268	3.833690	6.651989
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824740	1.274914
Cu	-1.803000	3.824740	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	5.099679	2.549827
Cu	0.000000	5.099679	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.435468	6.368728	3.875992
Cu	-1.776965	6.369187	3.875355
Cu	-5.418664	1.281824	3.866685
Cu	-1.793697	1.282512	3.867068
Cu	-5.417655	3.828336	3.815179
Cu	-1.795932	3.828565	3.806637
Cu	-3.606505	5.106870	4.974457
Cu	0.000072	5.105722	5.125535
Cu	-3.606721	0.002065	4.976752
Cu	-0.000793	0.021189	5.056307
Cu	-3.607298	2.556915	4.972673
Cu	0.001731	2.511554	5.100292

Table 20: Structure of the NH_2 →NH transition state (TS2), calculated at 0.167 ML in a (3×2) cell (Data for Fig. 16).

Element	x	y	z
H	-0.229774	5.312641	6.734476
H	1.204548	3.786340	7.041985
N	0.566719	3.739831	6.248351
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824740	1.274914
Cu	-1.803000	3.824740	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	5.099679	2.549827
Cu	0.000000	5.099679	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.424145	6.367810	3.846032
Cu	-1.766147	6.340961	3.877267
Cu	-5.411308	1.257039	3.837107
Cu	-1.785331	1.276010	3.820023
Cu	-5.430924	3.833843	3.907355
Cu	-1.791172	3.819768	3.800390
Cu	-3.589773	5.113219	4.983254
Cu	-0.017237	5.177781	5.258508
Cu	-3.599004	-0.003519	4.982234
Cu	-0.019184	-0.013081	5.017040
Cu	-3.596913	2.532284	4.972418
Cu	-0.022934	2.428404	5.120053

Table 21: Structure of the NH →N transition state (TS3), calculated at 0.167 ML in a (3×2) cell (Data for Fig. 16).

Element	x	y	z
H	-2.862371	3.825276	5.908842
N	-1.069035	3.825276	5.664696
Cu	-5.409000	1.274939	1.274914
Cu	-1.803000	1.274939	1.274914
Cu	-5.409000	3.824740	1.274914
Cu	-1.803000	3.824740	1.274914
Cu	-5.409000	6.374542	1.274914
Cu	-1.803000	6.374542	1.274914
Cu	-3.606000	2.549802	2.549827
Cu	0.000000	2.549802	2.549827
Cu	-3.606000	5.099679	2.549827
Cu	0.000000	5.099679	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.396019	6.347386	3.862733
Cu	-1.816486	6.381426	3.861586
Cu	-5.396163	1.302554	3.862988
Cu	-1.816631	1.267978	3.861076
Cu	-5.412750	3.824740	3.871912
Cu	-1.817568	3.825046	3.854191
Cu	-3.636290	5.093637	5.097487
Cu	0.020410	5.172349	5.093024
Cu	-3.622299	0.000000	4.985677
Cu	0.023872	0.000306	4.970888
Cu	-3.636074	2.556533	5.097614
Cu	0.020194	2.477973	5.092642

Table 22: Structure of the (2×2) 0.5 ML H2O/NH_3 phase (Data for Fig. 19, structure I).

Element	x	y	z
H	-4.437255	2.828268	12.68835
H	0.976144	0.632663	12.14146
H	-3.028896	3.662419	12.47437
H	-2.979998	2.034966	12.71466
H	0.268863	-0.735727	12.27609
N	-3.508349	2.784819	12.26589
O	0.192777	0.205210	12.54597
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.403735	1.285113	6.364164
Cu	-1.816703	1.285929	6.352537
Cu	-5.406115	3.817142	6.367224
Cu	-1.814539	3.815663	6.355801
Cu	-3.613861	0.008567	7.574007
Cu	-0.004327	0.005202	7.583390
Cu	-3.620064	2.565993	7.688239
Cu	-0.002596	2.547073	7.574210
Cu	-5.416212	3.850851	8.913380
Cu	-1.817063	3.840397	8.884210
Cu	-5.419457	1.309030	8.916439
Cu	-1.814756	1.312855	8.883189
Cu	-3.607659	0.035953	9.986143
Cu	-0.042551	0.041766	10.01225
Cu	-3.607659	2.589400	10.20033
Cu	-0.013775	2.615409	10.01001

Table 23: Structure of the (2×2) 1.0 ML H2O/NH_3 phase (Data for Fig. 19, structure II).

Element	x	y	z
H	-3.603043	2.577875	14.39041
H	-1.997003	2.241145	14.18132
H	0.330887	0.281552	14.85590
H	0.368389	1.084492	13.40720
H	-2.820036	3.134043	13.05552
H	-3.463563	1.035740	12.81053
H	-4.863628	0.506396	12.27528
H	0.689900	3.790777	13.15017
H	1.675348	3.120376	12.09964
H	-0.914914	0.108827	13.78600
N	-2.888767	2.345994	13.70236
N	0.094333	0.207760	13.86861
O	-3.919578	0.259725	12.32423
O	0.979750	2.908792	12.75464
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.409649	1.283838	6.392519
Cu	-1.802567	1.284144	6.395375
Cu	-5.408423	3.821630	6.390887
Cu	-1.803866	3.822344	6.392927
Cu	-3.599653	0.007904	7.694970
Cu	-0.003822	0.007700	7.609908
Cu	-3.601889	2.554264	7.609908
Cu	-0.006419	2.563647	7.666208
Cu	-5.411596	3.842997	8.939489
Cu	-1.795716	3.841467	8.967640
Cu	-5.413327	1.300514	8.942346
Cu	-1.794634	1.303829	8.981715
Cu	-3.590783	0.017798	10.20053
Cu	0.005193	0.032944	10.06121
Cu	-3.611264	2.587819	10.03897
Cu	0.008510	2.602557	10.17422

Table 24: Structure of the near-c(2×2) 1.0 ML H2O/NH_3 phase, calculated in a (2×2) cell (Data for Fig. 19, structure III).

Element	x	y	z
H	-4.601544	2.824546	12.62695
H	-2.122059	0.625779	14.91404
H	0.972250	3.250214	14.96626
H	0.274705	1.243245	12.41072
H	-3.203282	3.694751	12.52536
H	-3.135489	2.059393	12.71997
H	-3.551477	0.484722	14.34349
H	0.597514	-0.360444	12.64327
H	-0.113661	3.024656	13.86637
H	-0.976505	0.161608	12.52128
N	-3.647325	2.814550	12.25834
N	-0.026252	0.296953	12.17267
O	-2.609374	0.487017	14.07668
O	0.852675	3.026288	14.02242
Cu	-5.409000	1.274914	1.274914
Cu	-1.803000	1.274914	1.274914
Cu	-5.409000	3.824741	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	-3.606000	2.549827	2.549827
Cu	0.000000	2.549827	2.549827
Cu	-3.606000	0.000000	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-5.409000	3.824741	3.824741
Cu	-1.803000	3.824741	3.824741
Cu	-5.409000	1.274914	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	-3.606000	2.549827	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-3.606000	0.000000	5.099654
Cu	0.000000	0.000000	5.099654
Cu	-5.408423	1.291589	6.379668
Cu	-1.806173	1.292405	6.379056
Cu	-5.410010	3.828055	6.376812
Cu	-1.805019	3.826882	6.376607
Cu	-3.608885	0.018971	7.590529
Cu	-0.003390	0.019277	7.688035
Cu	-3.608957	2.578487	7.709658
Cu	-0.004039	2.575478	7.590938
Cu	-5.412678	3.865181	8.937042
Cu	-1.811150	3.857073	8.924191
Cu	-5.414481	1.313467	8.934186
Cu	-1.809058	1.318006	8.919908
Cu	-3.606577	0.039828	9.990630
Cu	-0.013703	0.037839	10.16932
Cu	-3.605711	2.595775	10.21889
Cu	-0.013486	2.618927	9.991038

Table 25: Structure of the (2×1) 1.0 ML H_2O/NH_3 phase (Data for Fig. 20, structure I).

Element	x	y	z
H	1.049021	-0.811355	12.38359
H	-0.686546	1.814712	13.11672
H	1.141155	0.765050	12.48660
H	-1.437135	2.429373	14.44712
H	-0.841713	3.424367	13.28786
N	-1.324556	2.540036	13.44126
O	0.515838	0.015503	12.36075
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.805019	1.278585	6.386399
Cu	-1.805272	3.824588	6.385583
Cu	-0.000541	0.003366	7.663557
Cu	0.002921	2.554723	7.604808
Cu	-1.809743	1.288887	8.954177
Cu	-1.809274	3.822293	8.955400
Cu	-0.012405	0.010709	10.15749
Cu	-0.011575	2.556814	10.06570

Table 26: Structure of the (2×1) 1.0 ML H_2O/NH_3 phase (Data for Fig. 20, structure II).

Element	x	y	z
H	0.836556	-0.405627	12.78341
H	0.269729	1.160681	12.71548
H	1.689375	0.766325	11.95502
H	-1.538680	2.796599	13.46778
H	-0.784990	3.111095	12.11943
N	0.754664	0.423118	12.19388
O	-0.673709	3.066473	13.10754
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.798024	1.271803	6.398230
Cu	-1.801089	3.831574	6.401290
Cu	0.015109	0.006069	7.729036
Cu	0.017056	2.560179	7.602565
Cu	-1.784321	1.308469	8.993955
Cu	-1.780967	3.873697	9.022716
Cu	0.020374	0.032791	10.30783
Cu	0.007609	2.612400	10.02918

Table 27: Structure of the (2×1) 1.0 ML H_2O/NH_3 phase (Data for Fig. 20, structure III).

Element	x	y	z
H	1.082161	-0.297973	12.94578
H	0.181165	1.109889	12.85521
H	1.478640	0.834405	11.82610
H	-1.671165	2.570532	12.82175
H	-0.484610	3.509072	13.06429
N	0.683589	0.396294	12.31016
O	-0.962550	2.760800	13.46696
Cu	-1.803000	1.274914	1.274914
Cu	-1.803000	3.824741	1.274914
Cu	0.000000	2.549827	2.549827
Cu	0.000000	0.000000	2.549827
Cu	-1.803000	3.824741	3.824741
Cu	-1.803000	1.274914	3.824741
Cu	0.000000	0.000000	5.099654
Cu	0.000000	2.549827	5.099654
Cu	-1.796978	1.274710	6.409041
Cu	-1.800043	3.821936	6.410265
Cu	0.004868	0.000153	7.739644
Cu	0.014208	2.544116	7.634794
Cu	-1.793769	1.288071	9.026388
Cu	-1.794850	3.832288	9.031896
Cu	-0.020158	-0.008414	10.31742
Cu	-0.003606	2.581700	10.09609