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Electronic Supplementary Information

Evidence for Efficient Anchoring in Nitroxyl Radical Thin Films: an Experimental XPS/NEXAFS and Theoretical DFT/TD-DFT Study

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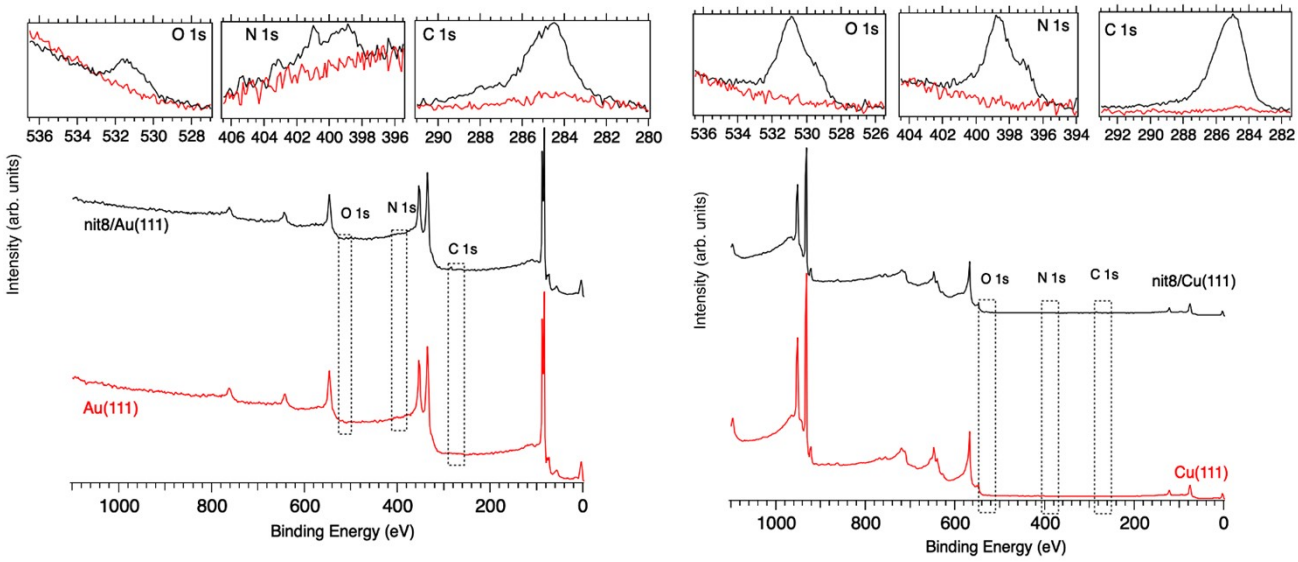

Figure S1: The overviews and core levels acquired before and after nit8 deposition on Au(111) and Cu(111) with *hv* = 1486.61 eV (Al K_α). After deposition, no further elements were detected besides O, N and C.

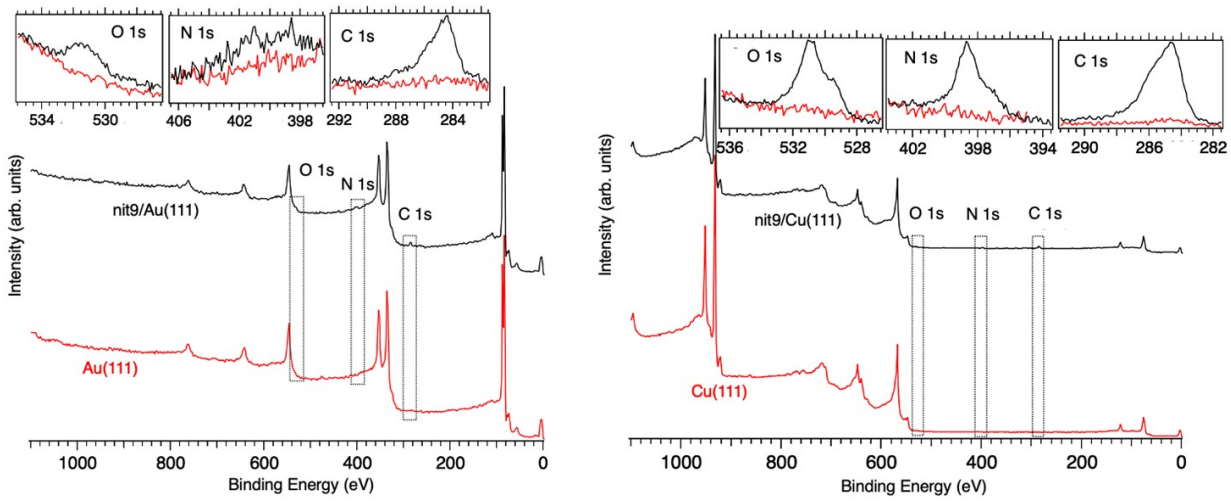

Figure S2: The overviews and core levels acquired before and after nit9 deposition on Au(111) and Cu(111) with *hv* = 1486.61 eV (Al K_α). After deposition, no further elements were detected besides O, N and C.

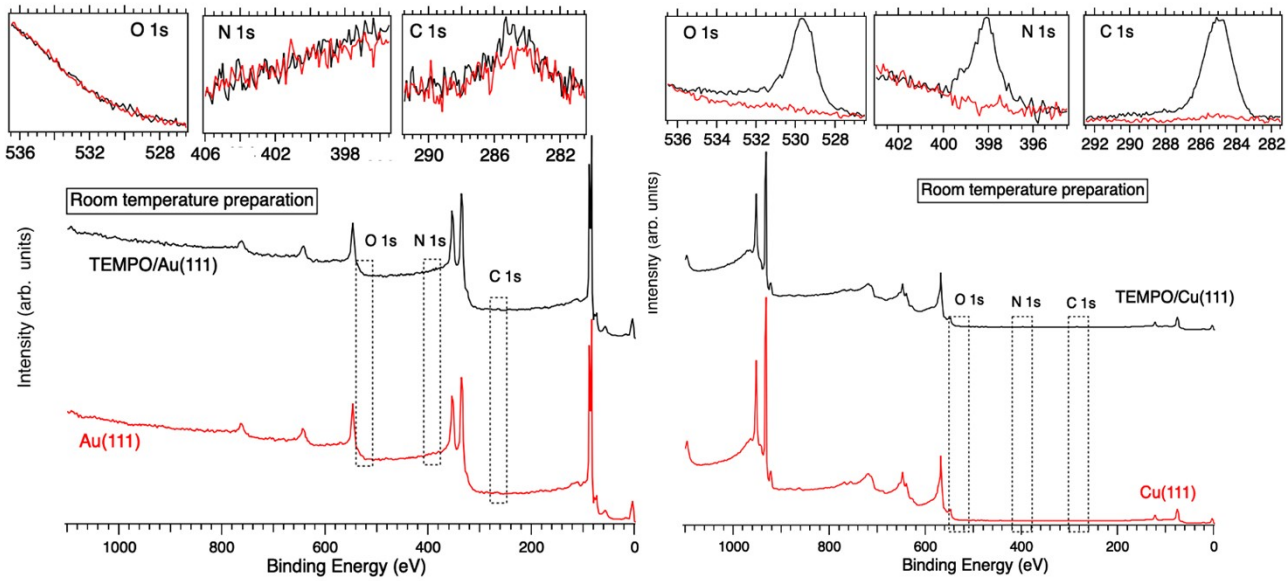

Figure S3: The overviews and core levels acquired before and after TEMPO deposition on Au(111) and Cu(111) with *hv* = 1486.61 eV (Al K_α). A proper and neat film was achieved on Cu(111) whereas no appreciable signal from TEMPO core levels could be detected on Au(111).

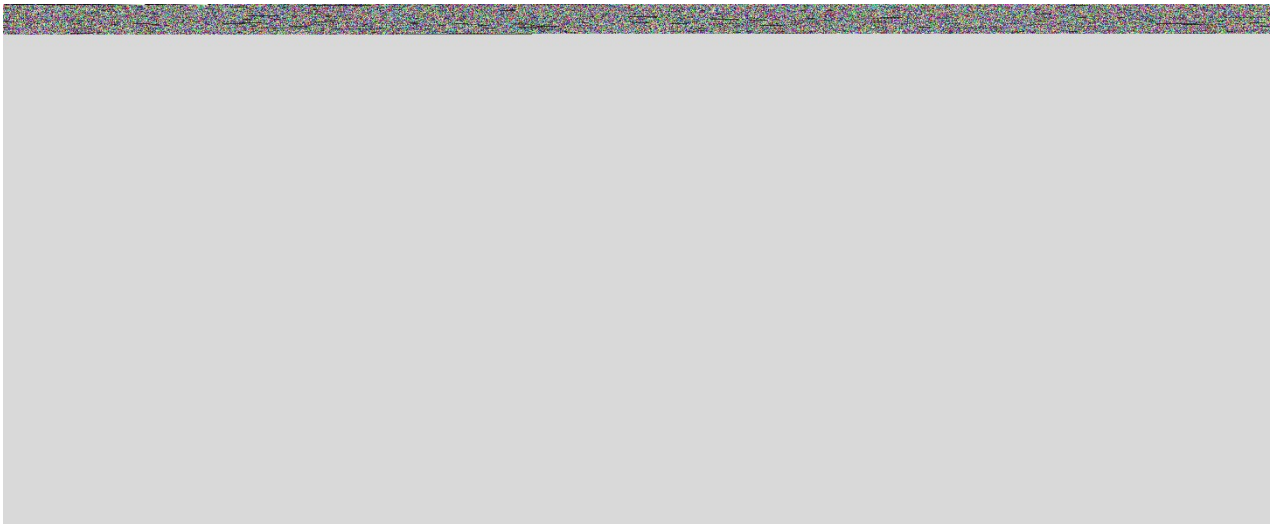

Figure S4: The overviews and core levels acquired before and after TEMPO deposition on Au(111) and Cu(111) cooled down by means of LN_2. The overview and O 1s: *hv* = 660 eV; N 1s and C 1s: *hv* = 515 eV. The preparation was successful on both substrates. After deposition no further elements were detected besides O, N and C. The Au 4f peaks are cut to allow O, N and C 1s spectra visualization.

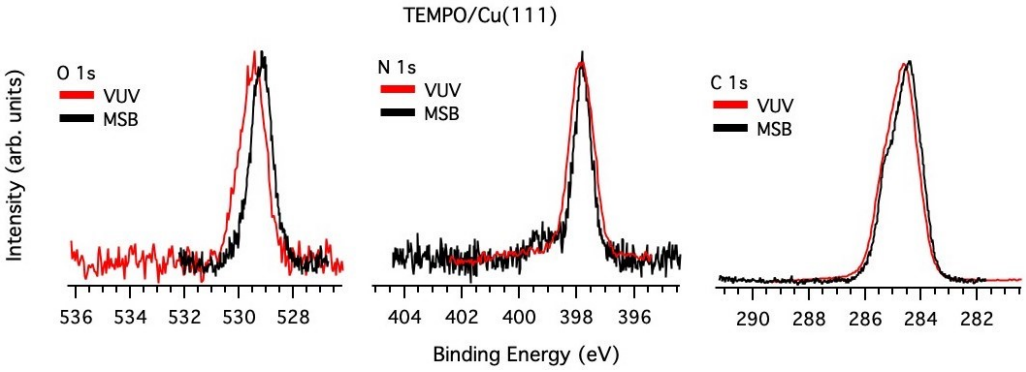

Figure S5. Comparison of TEMPO on Cu(111) XPS spectra as obtained at the VUV and MSB beamlines. At the VUV, the Cu substrate was cooled down by means of LN_2 whereas at the MSB, the film growth was performed at room temperature.

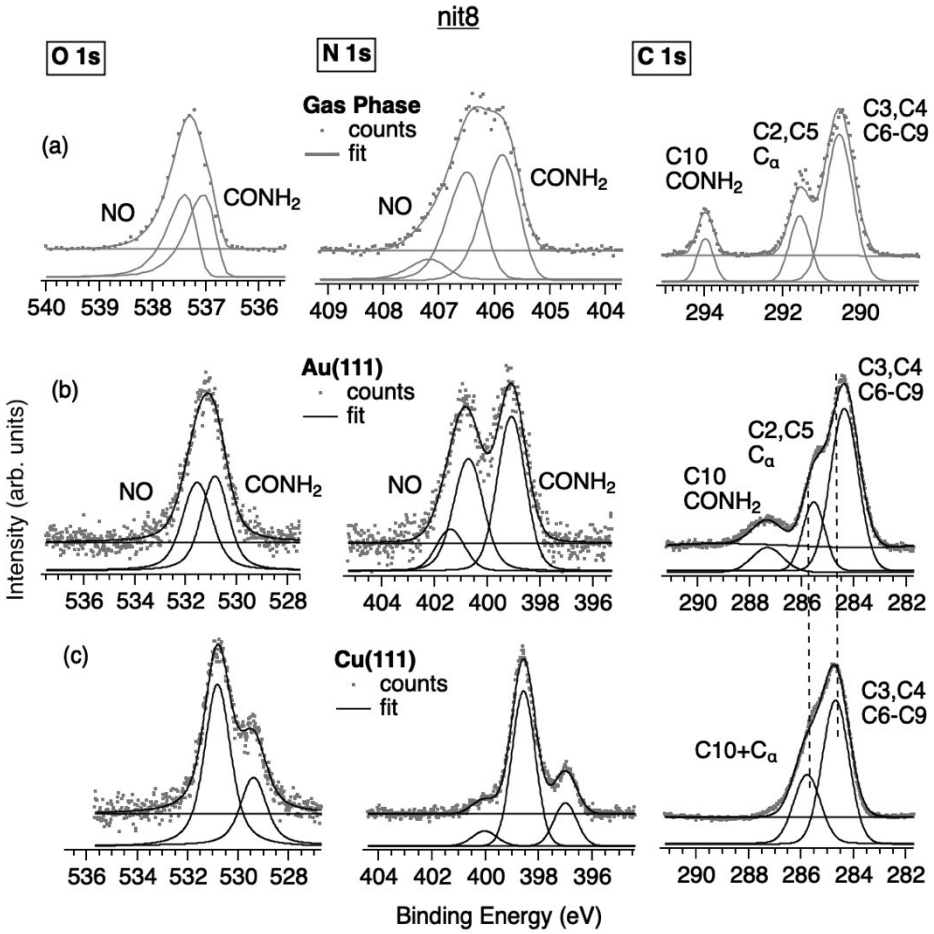

Figure S6. Comparison of nit8 O, N and C 1s core levels in (a) gas phase, and as thin films deposited onto the (b) Au(111) and (c) Cu(111) surface. For each spectrum, the fitting analysis is also shown. Note that different BE scales are employed to display the gas-phase and film results. Vertical dashed lines are added as a guide for better visualization of the peak alignment.

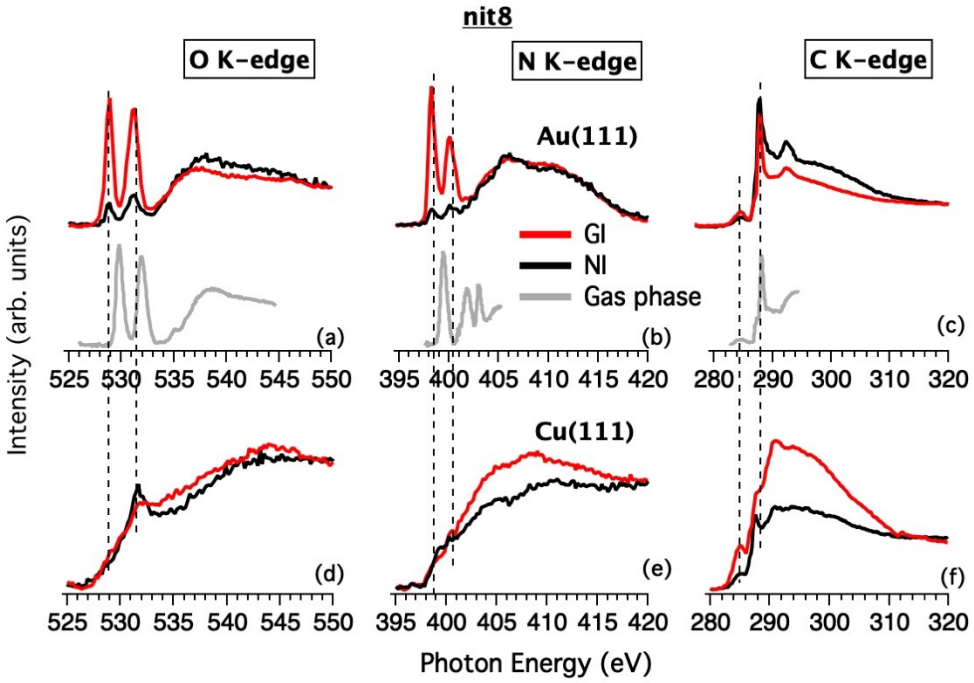

Figure S7. NEXAFS spectra of nit8 in the gas phase and adsorbed onto the Au(111) and Cu(111) surfaces at O K-edge (a and d), N K-edge (b and e) and C K-edge (c and f). Vertical dashed lines are added as line guide for a better visualization of peak alignment.

Table S1: Comparison between the BE positions (eV) of the C, N and O 1s core levels of nit8 and nit9 deposited on Au(111) and Cu(111) and the proposed spectral assignments: (i) **C_α** = C2 and C5, i.e. the C atoms bonded to N; (ii) **NO, $CONH_2$** is largely due to NO, with possibly a minor contribution due to $CONH_2$; (iii) **$CONH_2$ ⋯ Cu** is due to the fragments of $CONH_2$ on the Cu surface; (iv) **NO(*weak*)** is due to the S-T splitting in the final core-ionized states.

	Nit8 Nit9	Nit8 Nit9	Nit8 Nit9	Nit8 Nit9	Nit8 Nit9
C 1s	C10	C_α	C3, C4, C6-C9	Δ(C10 - C_α)	Δ(C_α - C3,C4,C6-C9)
Au(111)	287.3 287.6	285.5 285.8	284.4 284.5	1.8 1.8	1.1 1.3
Gas	294.0	291.6	290.5 290.4	2.4	1.1 1.2
N 1s	NO, NO(*weak*)	$CONH_2$		Δ(NO - $CONH_2$)	
Au(111)	400.7, 400.8, 401.4 401.4	399.1 398.7		1.6 2.1	
Gas	406.5, 406.7, 407.2 407.2	405.9		0.6 0.8	
O 1s	NO	$CONH_2$		Δ(NO - $CONH_2$)	
Au(111)	531.6 531.7	530.9 530.8		0.7 0.9	
Gas	537.2 537.3	536.8 536.9		0.4 0.4	
C 1s	C10	C_α	C3, C4,C6-C9	Δ(C10 - C_α)	Δ(C_α - C3,C4,C6-C9)
Cu(111)	- -	285.8 285.6	284.7 284.4	- -	1.1 1.2
N 1s	NO (*weak*)	NO, $CONH_2$	$CONH_2$ ⋯ Cu	Δ[(NO, $CONH_2$) - ($CONH_2$ ⋯ Cu)]	
Cu(111)	400.0 400.3	398.7 398.7	397.0 397.0	1.7 1.7	
O 1s	NO	NO, $CONH_2$	$CONH_2$ ⋯ Cu	Δ[(NO, $CONH_2$) - ($CONH_2$ ⋯ Cu)]	
Cu(111)	- -	530.8 530.7	529.4	1.4 1.3	

Table S2: The stoichiometry extracted from the XPS data of nit9 and nit8 on Au(111) and Cu(111).

nit9 ($C_9H_{15}N_2O_2$)	C (%)	N (%)	O (%)
Theoretical values	69.2	15.4	15.4
Au(111)	68.7	16.1	15.2
Cu(111)	74.1	13.8	12.1
nit8 ($C_9H_{17}N_2O_2$)	C (%)	N (%)	O (%)
Theoretical values	69.2	15.4	15.4
Au(111)	68.8	15	16.2
Cu(111)	72.4	15.1	12.6

Table S3: The stoichiometry extracted from the XPS data of TEMPO on Au(111) and Cu(111).

TEMPO	C (%)	N (%)	O (%)
Reference values	81.8	9.1	9.1
Au(111)	78	13	9
Cu(111)	78.5	13.5	8

Table S4: The XPS data fitting parameters. Gas phase spectra were simulated by employing Gaussian fit functions. A "shape" parameter was included in the fit, in order to obtain skewed curves.[1] These reproduced the characteristic asymmetric tail of gas phase photoemission peaks, due to the contribution of the intramolecular vibrations.[2,3,4] Differently from TEMPO, skewness was not needed for nit8 and nit9 C 1s gas phase spectra, where intramolecular vibrational modes get likely frustrated by the presence of the amide functional group. Peak positions and main spectral components were deduced from previous gas phase results.[5] Film data were simulated by employing Voigt fit functions. Considering the resemblance between gas phase and NRs/Au(111) results, for the film data the distances in BE between peaks, as well as the ratio between the peak areas, were kept fixed according to the gas phase values, while these constraints were kept slacker or not employed at all for Cu(111) data. For each peak, the Gaussian and the Lorenztian full width at half maximum (G. fwhm and L. fwhm, respectively) are indicated separately. Whenever possible, fwhm values were constrained to have the same value for the components of the same spectrum.

Nit8

Gas phase

Core level	Peak	BE (eV)	G. fwhm (eV)	Shape parameter
C 1s	C 10	294	0.5	-
	C_α	291.6	0.6	-
	C3, C4, C6 – C9	290.5	0.8	-
N 1s	NO (weak)	407.2	0.8	0.2
	NO	406.5	0.8	0.2
	$CONH_2$	405.9	0.8	0.2
O 1s	NO	537.2	0.7	0.4
	$CONH_2$	536.8	0.7	0.4

Au(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C 1s	C 10	287.3	1.4	-
	C_α	285.5	1.0	-
	C3, C4, C6 – C9	284.4	1.3	-
N 1s	NO (weak)	401.4	1.2	0.3
	NO	400.7	1.2	0.3
	$CONH_2$	399.1	1.2	0.3
O 1s	NO	531.6	1.1	0.5
	$CONH_2$	530.9	1.0	0.5

Cu(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C1s	C_α	285.8	1.1	0.1
	C3, C4, C6 – C9	284.7	1.1	0.1
N 1s	NO (weak)	400.0	0.7	0.5
	NO, $CONH_2$	398.7	0.7	0.5
	$CONH_2$ ··· Cu	397.0	0.7	0.5
O 1s	NO, $CONH_2$	530.8	0.8	0.7
	$CONH_2$ ··· Cu	529.4	0.8	0.7

Nit9

Gas phase

Core level	Peak	BE (eV)	G. fwhm (eV)	Shape parameter
C 1s	C 10	294.0	0.5	-
	C_α	291.6	0.6	-
	C3, C4, C6 – C9	290.4	0.8	-
N 1s	NO (weak)	407.2	0.8	0.2
	NO	406.7	0.6	0.2
	$CONH_2$	405.9	0.7	0.2
O 1s	NO	537.3	0.7	0.2
	$CONH_2$	536.9	0.7	0.3

Au(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C 1s	C 10	287.6	0.9	0.4
	C_α	285.8	0.7	0.4
	C3, C4, C6 – C9	284.5	0.9	0.4
N 1s	NO (weak)	401.4	0.5	0.5
	NO	400.7	0.5	0.4
	$CONH_2$	398.7	0.9	0.3
O 1s	NO	531.7	0.7	0.6
	$CONH_2$	530.8	0.7	0.6

Cu(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C 1s	C 10	287.6	0.9	0.4
	C_α	285.8	0.7	0.4
	C3, C4, C6 – C9	284.5	0.9	0.4
N 1s	NO (weak)	401.4	0.5	0.5
	NO	400.7	0.5	0.4
	$CONH_2$	398.7	0.9	0.3
O 1s	NO	531.7	0.7	0.6
	$CONH_2$	530.8	0.7	0.6

TEMPO

Gas phase

Core level	Peak	BE (eV)	G. fwhm (eV)	Shape parameter
C 1s	C2, C6	291.3	0.5	0.2
	C4	290.7	0.5	0.2

	C8, C9, C3, C5	290.4	0.5	0.2
	C7, C10	290.1	0.5	0.2
N 1s	NO	406.4	0.6	0.2
	NO (weak)	407.0	0.6	0.2
O 1s	NO	537.0	0.6	0.3

Au(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C 1s	C_α	285.5	1.0	0.1
	C3-C5, C7-C10	284.3	1.0	0.3
N 1s	NO	400.8	1.1	0.3
O 1s	NO	531.4	1.0	0.2

Cu(111)

Core level	Peak	BE (eV)	G. fwhm (eV)	L. fwhm (eV)
C 1s	C_α	285.2	0.9	0.1
	C3-C5, C7-C10	284.3	1.0	0.1
N 1s	NO	397.8	0.8	0.2
O 1s	NO	529.5	1.1	0.0

Additional computational details

Siesta. Siesta[6] is a first-principles periodic DFT code and method that combines the norm-conserving pseudopotential approach with linearly combined atomic-centred orbitals (LCAO) basis functions of finite support, i.e. each AO is exactly zero beyond a chosen cut-off radius. This method was used for the fully unconstrained optimizations of the unit cells consisting of one NR molecule adsorbed on a 3-layer 4 × 4 Cu (111) or 4-layer 3 × 3 Au (111) slab. Taking care that the minimum distance of the adsorbates from neighbouring unit cells is not unphysically small, we found that the 4 × 4 Cu and 3 × 3 Au unit cells with one adsorbed NR molecule (i.e. 1/16 and 1/9 coverages) are of suitable size to represent the fully saturated NR monolayers on the Cu (lattice constant 3.6 Å) and Au (lattice constant 4.1 Å) slabs, in accordance with the experimental conditions. For these large and computationally expensive unit cells, the *k*-point grid cut-off parameter[7] was limited to 10 Å, which gave rise to 5 k-points for the Au slabs, and 2 k-points for the larger Cu slabs. The vacuum space between the apex atom of NR and the lowest layer of the metal slab was always kept larger than 11 Å, which was sufficient to prevent undesired artificial interactions between the adjacent slab copies.

For the exchange-correlation (XC) density functional, we used the Hammer-Hansen-Nørskov revised version of the generalized gradient approximation (GGA) XC functional of Perdew, Burke, and Ernzerhof (PBE), denoted by RPBE.[8] Relative to PBE, the RPBE functional resulted in the improved adsorption energies on metal surfaces while also rectifying certain deficiencies in the earlier proposed Zhang-Yang revision of PBE.[9] The double-ζ polarized (DZP) basis sets of the hard-confined numerical orbitals of the Sankey–Niklewski type were used in all cases.[10]

Using the auxiliary program Atom 4.2.0 supplied with Siesta, we generated hard pseudopotentials (PPs) of the improved Troullier–Martins flavor[11,12] for the H, C, N, O, Cu, and Au atoms based on the RPBE functional.[8] The PPs were non-relativistic for H, C, N, and O, and relativistic and in addition core-corrected[13] for Cu and Au. The thus-generated PPs showed a good transferability in the subsequently performed tests with various electron configurations. The excitation energy determining the orbital confinement radii[14] (the PAO.EnergyShift parameter in Siesta) was set to 0.01 Ry, which allowed for the more extended atomic orbitals than the default value of 0.02 Ry. We observed this parameter to be crucial for satisfactorily reproducing the lattice constants and cohesive energies of the Cu and Au bulk metals. The plane wave equivalent energy cut-off for the 3D grid was set to 300 Ry, which was sufficient to curb the numerical noise due to the “egg-box” effect (the oscillations in the energy and forces when translating the atoms in the unit cell). The electronic temperature for the Fermi-Dirac smearing during the SCF procedure was set to 300 K; hence the reported adsorption energies concern the differences in the electronic free energies.[15] The periodic calculations on the unit cells containing NRs (i.e. the NR adsorbed on the surface as well as the bare radical) were performed as spin-polarized (the collinear polarization) with the spin value fixed at 1.0 (doublet) while those containing only the metal slabs were spin-non-polarized.

The FIRE[16] and modified Broyden search algorithms were used interchangeably during the geometry optimizations. All the atoms in the unit cells together with the lattice vectors were allowed to relax until the forces on each atom fell below 0.05-0.06 eV/Å, corresponding to <0.01 eV accuracy in the final energies. This is sufficient for the purpose of obtaining a set of reasonable structures for the subsequent single-point DFT and TD-DFT computations using the Orca code.

The obtained final energies were used to compute the adsorption energies (E_{ads}) of the two NRs on the Cu and Au surfaces for the various tested adsorption sites according to:

$$E_{ads} = E(\text{NR}\cdots\text{slab}) - (E(\text{NR}) + E(\text{slab})) \quad (1)$$

All the energy terms pertain to the fully relaxed unit cells. In the optimization of the isolated NR molecules, for the starting lattice vectors we used the final lattice vectors from the corresponding NR···slab unit cell and retained the same *k*-grid cut-off parameter.

Orca. We next switched to the Orca[17,18] code, version 5.0.3, and all-electron basis sets to retrieve the information about the C, N, and O 1s core electrons. To this end, single-point DFT and restricted single excitation space (RSES) TD-DFT computations[19] were performed for the structures consisting of one NR molecule bonded onto two-layer Cu or Au clusters. These structures are cut-out portions of the Siesta optimized unit cells, and were used as such without further optimization. For the DFT and RSES-TD-DFT single-point calculations, the long-range corrected hybrid CAM-B3LYP density functional[20] was used, which showed superior performance for the diffuse and charge-transfer excited states relative to the parent B3LYP.[20] To describe the scalar relativistic effects important for the transition metal atoms, the zeroth-order regular approximation (ZORA) was employed.[21] For the H, C, N, O, and Cu atoms we used the re-contracted versions of the all-electron Karlsruhe def2-TZVP basis sets[22,23] suitable for ZORA computations, and denoted by ZORA-def2-TZVP, while SARC-ZORA-TZVP was used for the Au atoms.[24] For the systems of TEMPO (nit9) adsorbed on the 14-atom Cu or Au cluster this choice led to 1230 (1276) and 2014 (2060) basis functions, respectively. The preliminary tests indicated only a minor effect of adding the diffuse functions via the minimal augmentation (ma-), and so to save time we omitted them from the basis set. To speed-up these expensive calculations by means of the density fitting, the segmented all-electron relativistically contracted (SARC) Coulomb-fitting auxiliary sets were adopted, denoted by SARC/J. Also, the RIJCOSX approach was used whereby the Coulomb term is evaluated using the resolution of identity (RI) approximation while the exchange term is evaluated via the semi-numerical ("chain-of-spheres") integration.[25,26] The used Orca tight "DEFGRID3" DFT integration grid consisted of the M3-mapped Gauss-Chebyshev radial grids and 302-points Lebedev angular grids resulting on average in ca. 7,000 (11,000) grid points per atom for the Cu (Au) clusters. The reason for using the simple Koopmans' approximation to model the XPS spectra instead of the preferred ΔDFT approach, which allows for the orbital relaxation effects, is that the core-hole states were found to be unfeasibly difficult to converge for the systems of this complexity.

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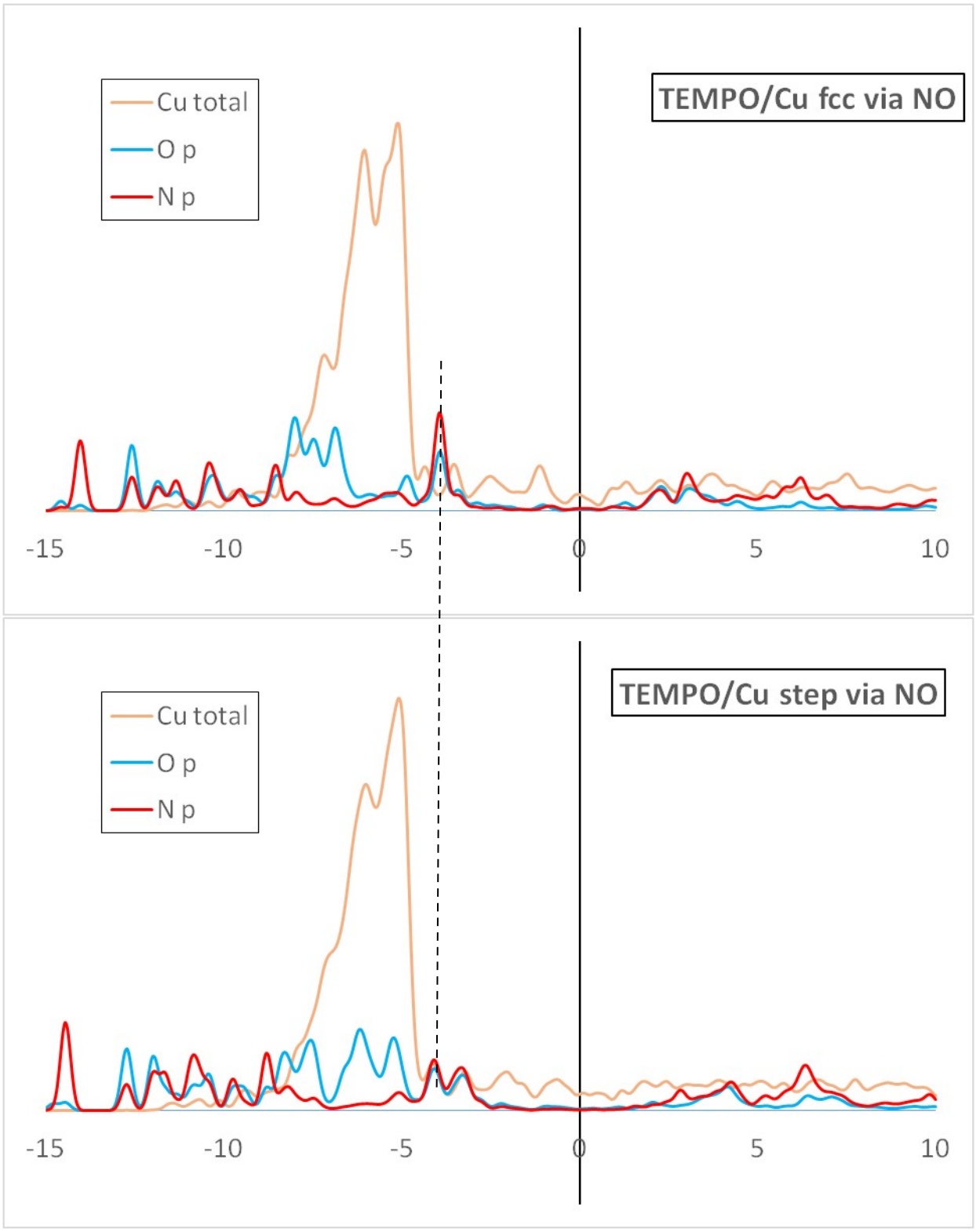


Figure S8. Partial density of states (PDOS) plots (energy in eV) for the two types of adsorption in the TEMPO/Cu system (O p = 2*p*-orbitals on the O atom etc.). The π(N-O) spike (dashed vertical rule) is higher in case of the adsorption on the flat Cu owing to the larger charge donation from the Cu surface.

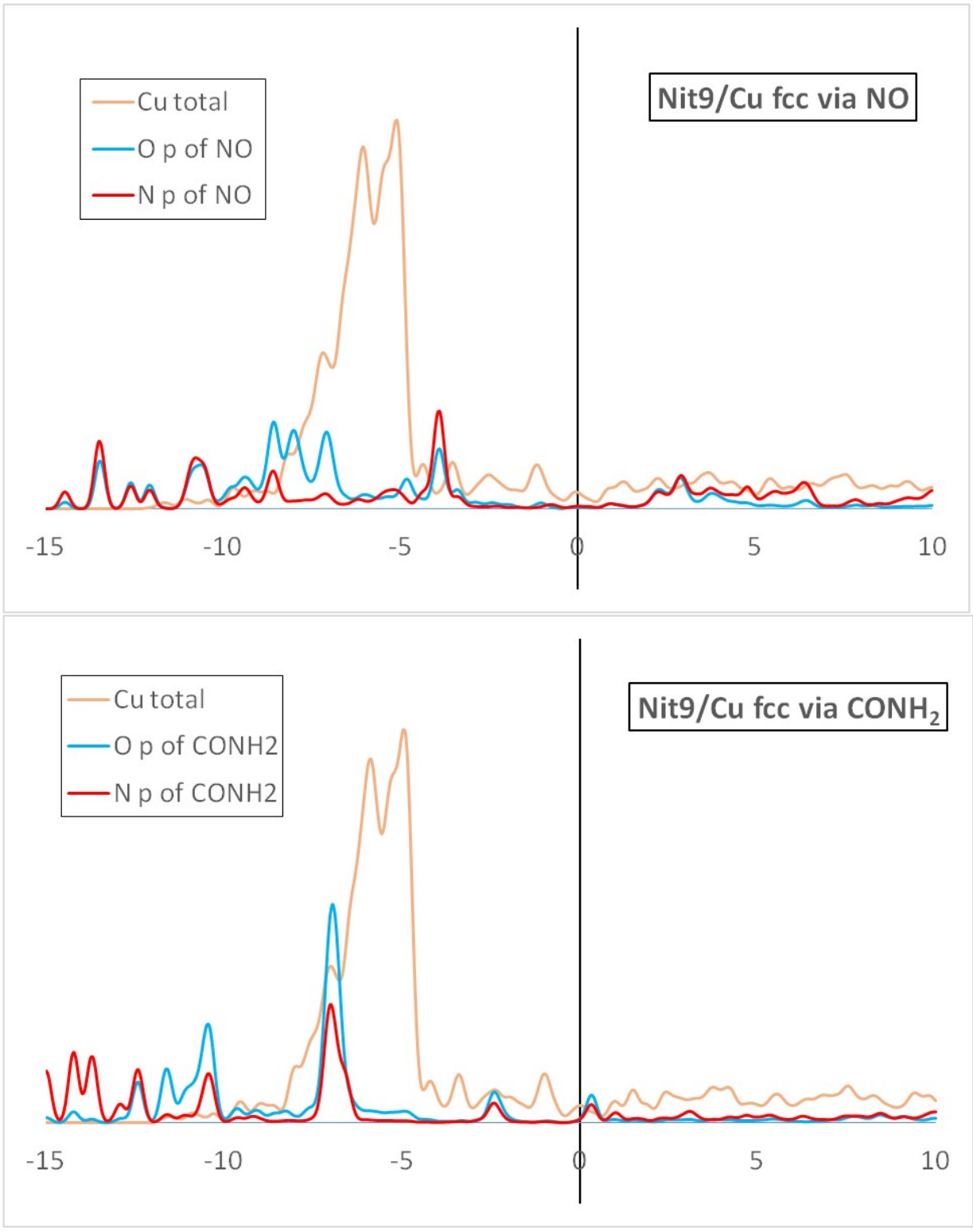


Figure S9. Partial density of states (PDOS) plots (energy in eV) for the two types of adsorption in the nit9/Cu system (O p = 2*p*-orbitals on the O atom etc.). The interaction of the NO and $CONH_2$ 2*p* states with the Cu surface states is clearly visible in both cases.

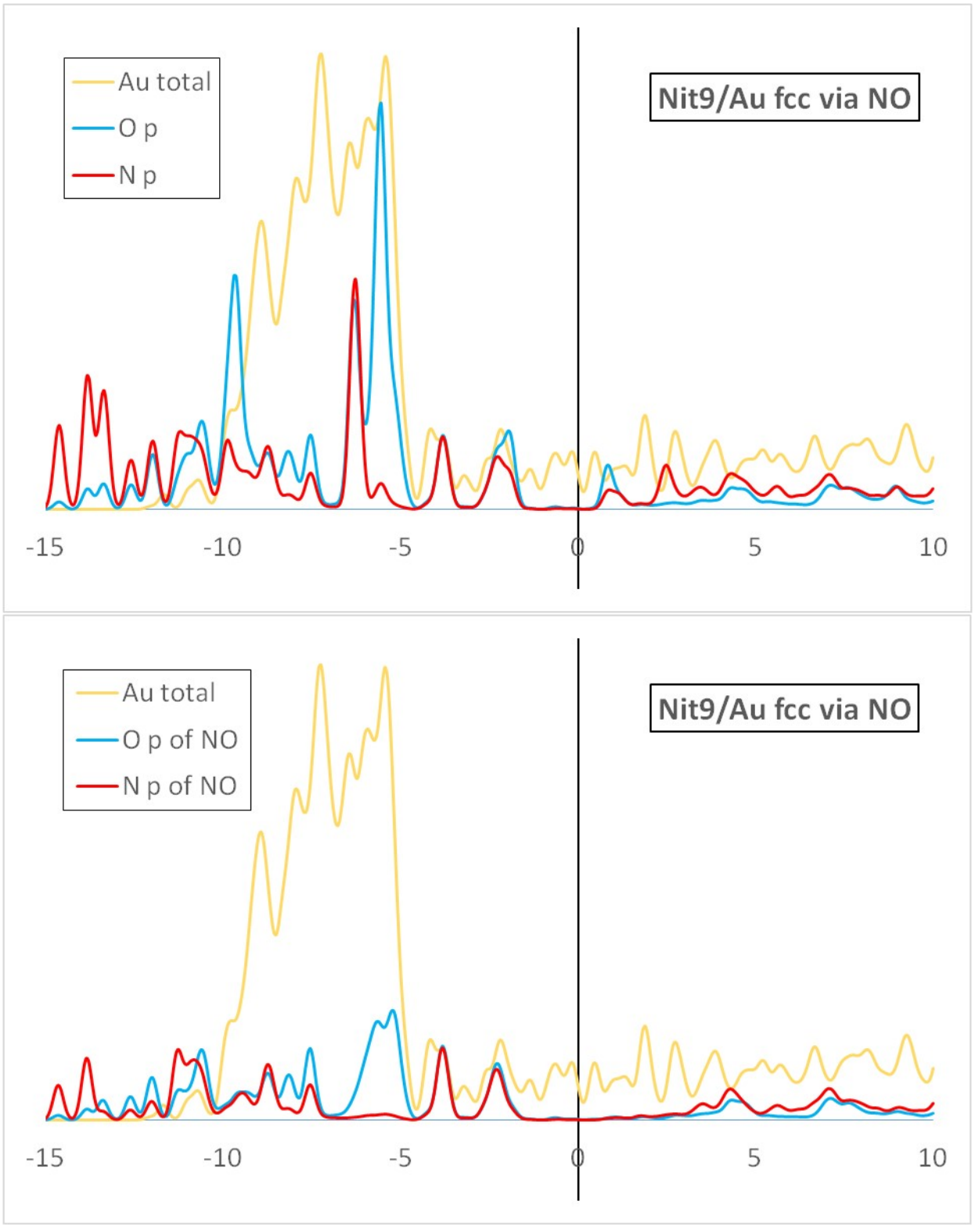


Figure S10. Partial density of states (PDOS) plots (energy in eV) for the adsorption of nit9 via the NO group onto the flat Au(111) surface. The upper panel shows the total (NO + $CONH_2$) 2*p* states, and the lower panel only the 2*p* states of the NO group.

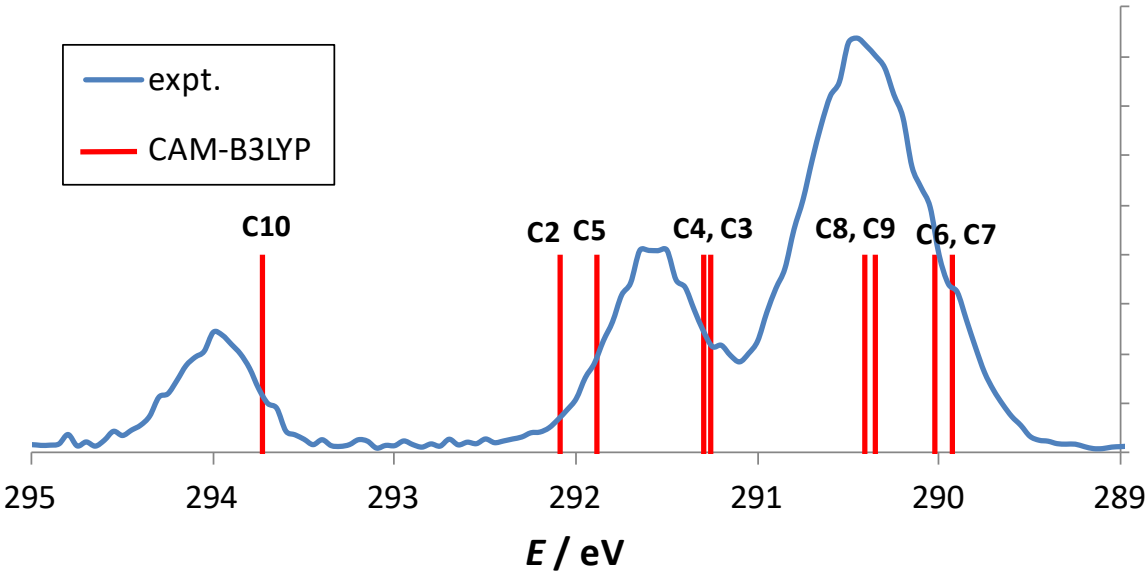


Figure S11. The calibration of the computational methods against the experimental gas phase C 1s XPS spectrum of nit9 (blue line). The red vertical rules show the positions of the CAM-B3LYP/ZORA-def2-TZVP C 1s orbital energies (the β spin set) with the numbering of the C atoms according to Figure 1. The orbital energies are shifted upwards by 11 eV.

Table S5. The calibration of the computational methods against the experimental gas phase N 1s and O 1s XPS spectra of nit9. The CAM-B3LYP/ZORA-def2-TZVP N 1s and O 1s orbital energies (the β spin set in eV) are given; Δ = difference between the N and O atoms of the $CONH_2$ and NO groups.

N 1s XPS expt.		**Δ expt.**	**CAM-B3LYP/ ZORA-def2-TZVP**		**Δ calc.**
$CONH_2$	**NO**		**$CONH_2$**	**NO**	
405.9	406.7	0.8	-393.1347	-394.2605	1.1
O 1s XPS expt.					
536.9	537.3	0.4	-522.8794	-523.1376	0.3

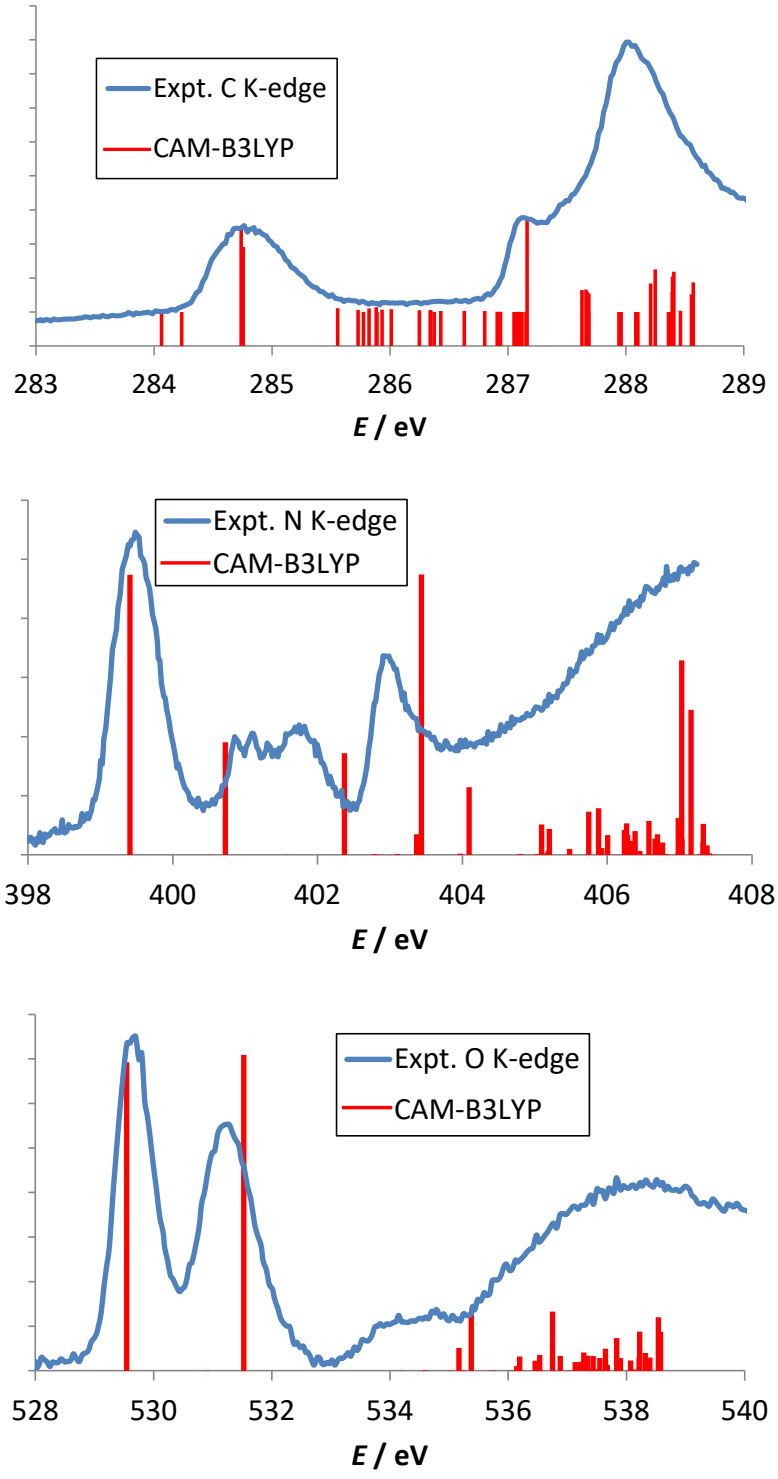


Figure S12. The calibration of the computational methods against the experimental gas phase NEXAFS spectra of nit9 (blue lines). The red vertical rules show the positions of the TD-CAM-B3LYP/ZORA-def2-TZVP excitation energies and oscillator strengths. The excitation energies were shifted upwards by 10.2 eV (C 1s), 12.2 eV (N 1s), and 13.8 eV (O 1s).

Table S6. The Voronoi charges for the nit9/Cu system and different modes of adsorption (Δ = difference in charges on O or N atoms with respect to the isolated nit9: "+" sign = nit9 donates the charge to the surface; "–" sign = nit9 accepts the charge from the surface)

		FLAT			STEP		
O atoms	**nit9**	**hcp**	**fcc**	**CO**	**CO**	**NO**	**NH_2**
NO	-0.214	-0.264	-0.264	-0.219	-0.220	-0.234	-0.211
$CONH_2$	-0.265	-0.262	-0.263	-0.253	-0.230	-0.264	-0.242
Δ(NO)		-0.050	-0.050	-0.005	-0.006	-0.020	0.003
Δ($CONH_2$)		0.003	0.002	0.012	0.035	0.001	0.023
N atoms							
NO	0.096	-0.005	-0.002	0.094	0.096	0.087	0.094
$CONH_2$	-0.118	-0.122	-0.115	-0.099	-0.100	-0.115	-0.099
Δ(NO)		-0.101	-0.098	-0.002	0.000	-0.009	-0.002
Δ($CONH_2$)		-0.004	0.003	0.019	0.018	0.003	0.019

Table S7. The Voronoi charges for the nit9/Au system and different modes of adsorption (Δ = difference in charges on O or N atoms with respect to the isolated nit9: "+" sign = nit9 donates the charge to the surface; "–" sign = nit9 accepts the charge from the surface)

O atoms	**nit9**	**hcp**	**fcc**	**CO**	**recline**
NO	-0.212	-0.231	-0.231	-0.231	-0.198
$CONH_2$	-0.268	-0.265	-0.268	-0.276	-0.271
Δ(NO)		-0.019	-0.019	-0.019	0.014
Δ($CONH_2$)		0.003	0.000	-0.008	-0.003
N atoms					
NO	0.095	0.110	0.111	0.097	0.111
$CONH_2$	-0.118	-0.117	-0.116	-0.107	-0.115
Δ(NO)		0.015	0.016	0.002	0.016
Δ($CONH_2$)		0.001	0.002	0.011	0.003

Table S8. Mulliken spin densities on the N and O atoms for the nit9/Cu system and different modes of adsorption (Δ = difference between the α and β spin densities)

	nit9					**hcp NO**			
	NO		$CONH_2$			NO		$CONH_2$	
	N	O	N	O		N	O	N	O
α	2.675	3.310	2.216	3.017		2.467	3.131	2.212	3.017
β	2.239	2.812	2.215	3.017		2.467	3.129	2.211	3.017
Δ	**0.436**	**0.498**	**0.001**	**0.000**		**0.000**	**0.002**	**0.001**	**0.000**
	fcc NO					**flat $CONH_2$**			
	NO		$CONH_2$			NO		$CONH_2$	
	N	O	N	O		N	O	N	O
α	2.461	3.133	2.212	3.017		2.676	3.313	2.194	3.013
β	2.457	3.130	2.212	3.017		2.245	2.814	2.194	3.013
Δ	**0.004**	**0.003**	**0.000**	**0.000**		**0.431**	**0.499**	**0.000**	**0.000**
	step CO					**step NO**			
	NO		$CONH_2$			NO		$CONH_2$	
	N	O	N	O		N	O	N	O
α	2.675	3.311	2.193	3.010		2.622	3.213	2.212	3.016
β	2.237	2.817	2.193	3.009		2.247	2.928	2.212	3.016
Δ	**0.438**	**0.494**	**0.000**	**0.001**		**0.375**	**0.285**	**0.000**	**0.000**
	step NH_2								
	NO		$CONH_2$						
	N	O	N	O					
α	2.674	3.309	2.249	3.000					
β	2.240	2.810	2.249	3.000					
Δ	**0.434**	**0.499**	**0.000**	**0.000**					

Table S9. Mulliken spin densities on the N and O atoms for the nit9/Au system and different modes of adsorption (Δ = difference between the α and β spin densities)

	nit9					**hcp NO**			
	NO		$CONH_2$			NO		$CONH_2$	
	N	O	N	O		N	O	N	O
α	2.674	3.310	2.215	3.019		2.670	3.263	2.212	3.019
β	2.238	2.811	2.215	3.019		2.216	2.832	2.212	3.018
Δ	**0.436**	**0.499**	**0.000**	**0.000**		**0.454**	**0.431**	**0.000**	**0.001**
	fcc NO					**flat $CONH_2$**			
	NO		$CONH_2$			NO		$CONH_2$	
	N	O	N	O		N	O	N	O
α	2.669	3.261	2.212	3.019		2.678	3.317	2.201	3.004
β	2.217	2.834	2.212	3.018		2.233	2.828	2.201	3.004
Δ	**0.452**	**0.427**	**0.000**	**0.001**		**0.445**	**0.489**	**0.000**	**0.000**
	parallel								
	NO		$CONH_2$						
	N	O	N	O					
α	2.670	3.281	2.215	3.022					
β	2.216	2.826	2.215	3.022					
Δ	**0.454**	**0.455**	**0.000**	**0.000**					

Table S10. The computed (TD-CAM-B3LYP/ZORA-def2-TZVP) C, N, and O 1s core-excited spectra (the excitation energies and corresponding oscillator strengths (*f*)) of the gas-phase monomer (M) and dimer (D) of nit9. The key difference is seen in the O 1s spectra (highlighted in red) where the strongest excitations to π^*(NO) and π^*($CONH_2$) are by 0.22 eV more separated in the dimer than in the monomer.

C 1s				**N 1s**				**O 1s**			
M	***f***	**D**	***f***	**M**	***f***	**D**	***f***	**M**	***f***	**D**	***f***
273.803	0.00	273.810	0.00	387.310	0.02	387.309	0.02	515.819	0.03	515.821	0.02
273.985	0.00	273.810	0.00	388.407	0.00	387.309	0.03	517.168	0.00	515.821	0.03
274.484	0.07	274.001	0.00	388.616	0.01	387.984	0.00	517.793	0.03	517.477	0.00
274.494	0.00	274.001	0.00	389.430	0.00	387.985	0.00	520.464	0.00	517.477	0.00
275.335	0.00	274.492	0.04	390.201	0.01	388.241	0.01	520.852	0.00	518.020	0.00
275.497	0.00	274.493	0.07	390.692	0.00	388.241	0.02	520.852	0.00	518.020	0.04
275.540	0.00	274.514	0.01	390.701	0.00	389.610	0.00	521.173	0.00	520.504	0.00
275.590	0.00	274.514	0.02	391.005	0.00	389.610	0.00	521.322	0.00	520.504	0.00
275.679	0.00	275.370	0.00	391.224	0.02	390.293	0.02	521.450	0.00	520.565	0.00
275.694	0.00	275.370	0.00	391.284	0.01	390.293	0.01	521.598	0.01	520.565	0.00

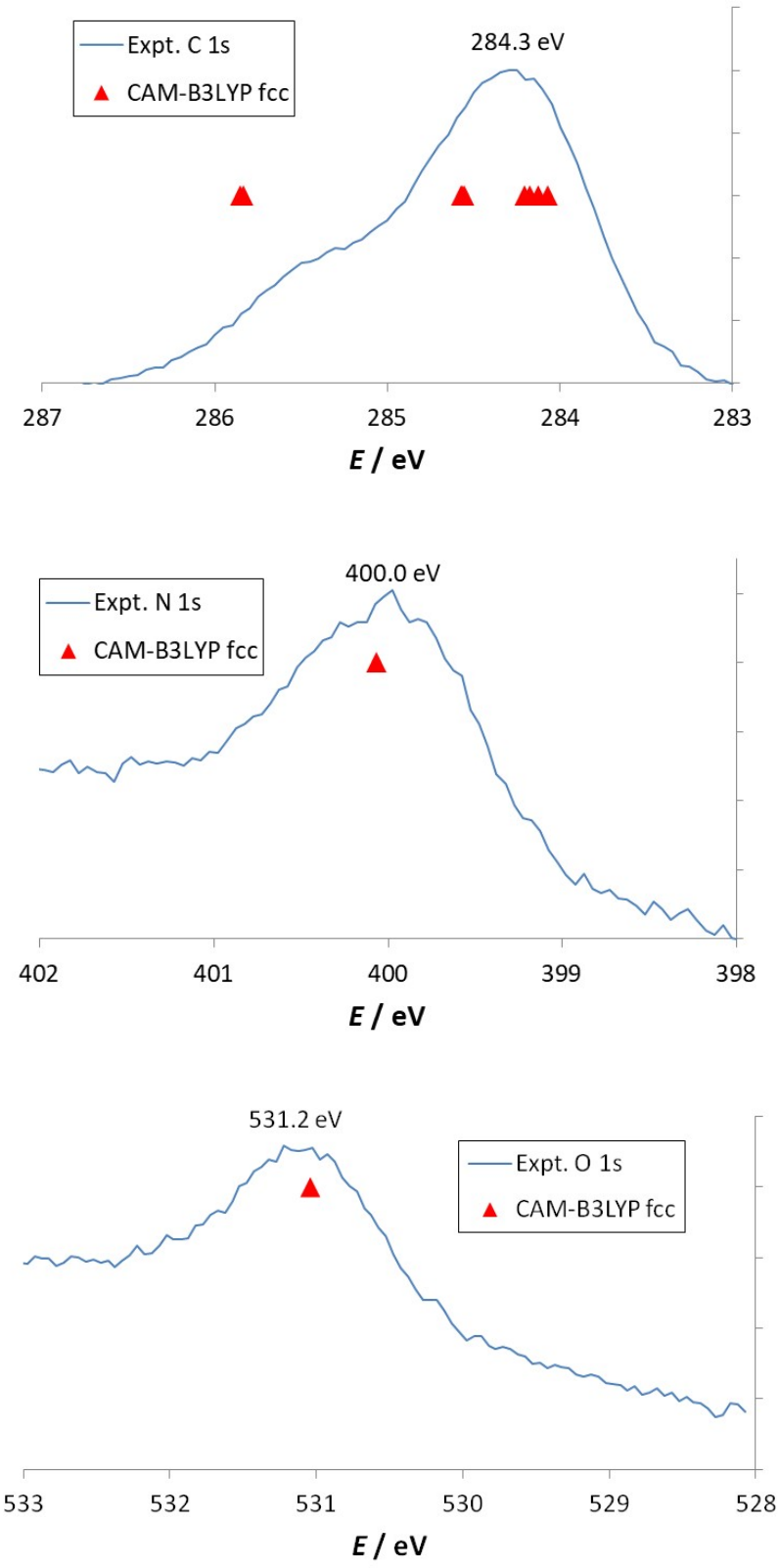


Figure S13. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) XPS spectra of the TEMPO/Au system (fcc = adsorption via NO on the flat surface above the fcc site). The upward energy shifts of 5.0 (C 1s), 5.4 (N 1s), and 7.5 eV (O 1s) were applied for the modelled spectra.

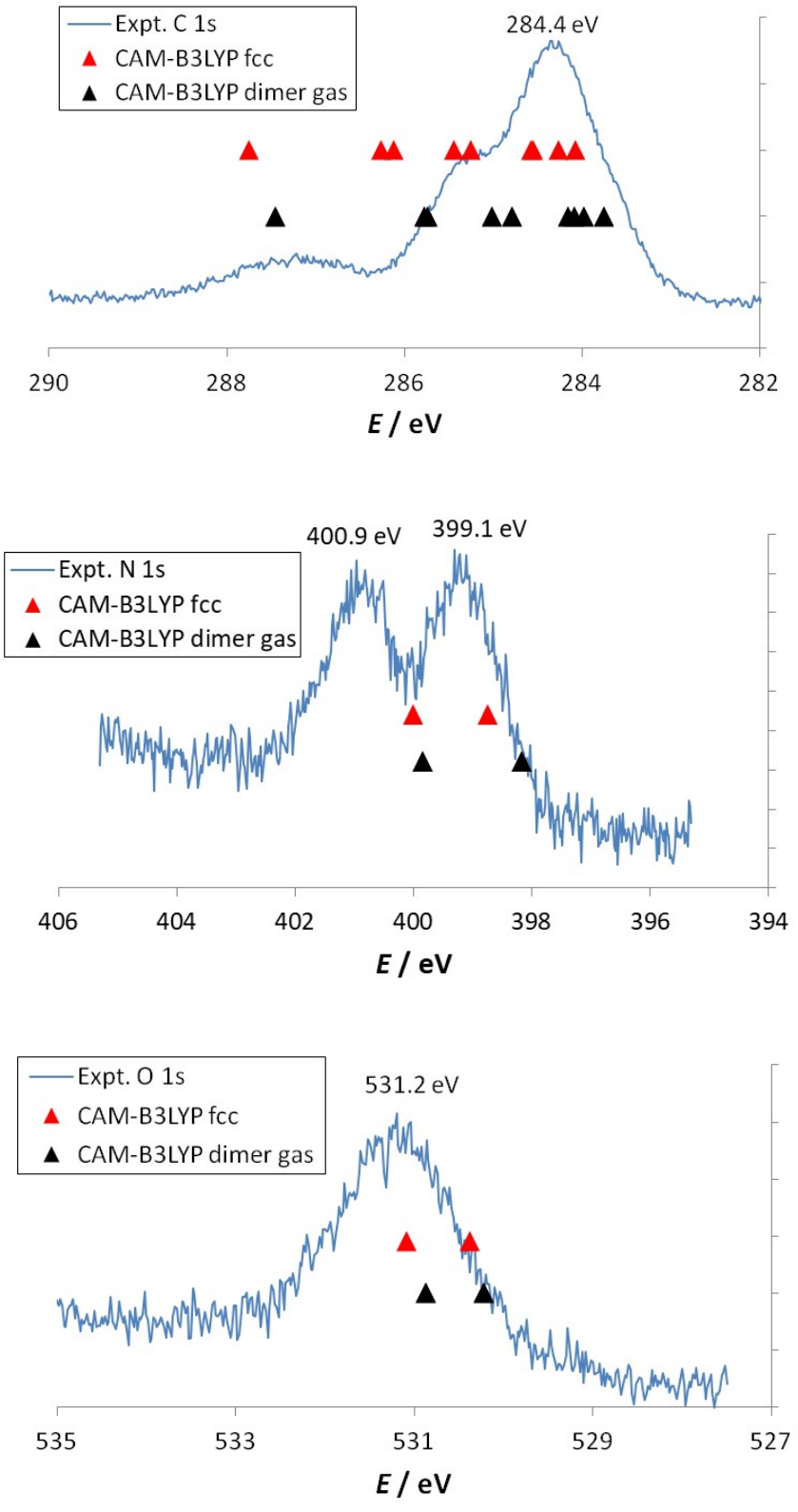


Figure S14. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) XPS spectra of the nit8/Au system (fcc = adsorption via NO on the flat surface above the fcc site). The upward energy shifts of 5.0 (C 1s), 5.4 (N 1s), and 7.5 eV (O 1s) were applied for the modelled spectra.

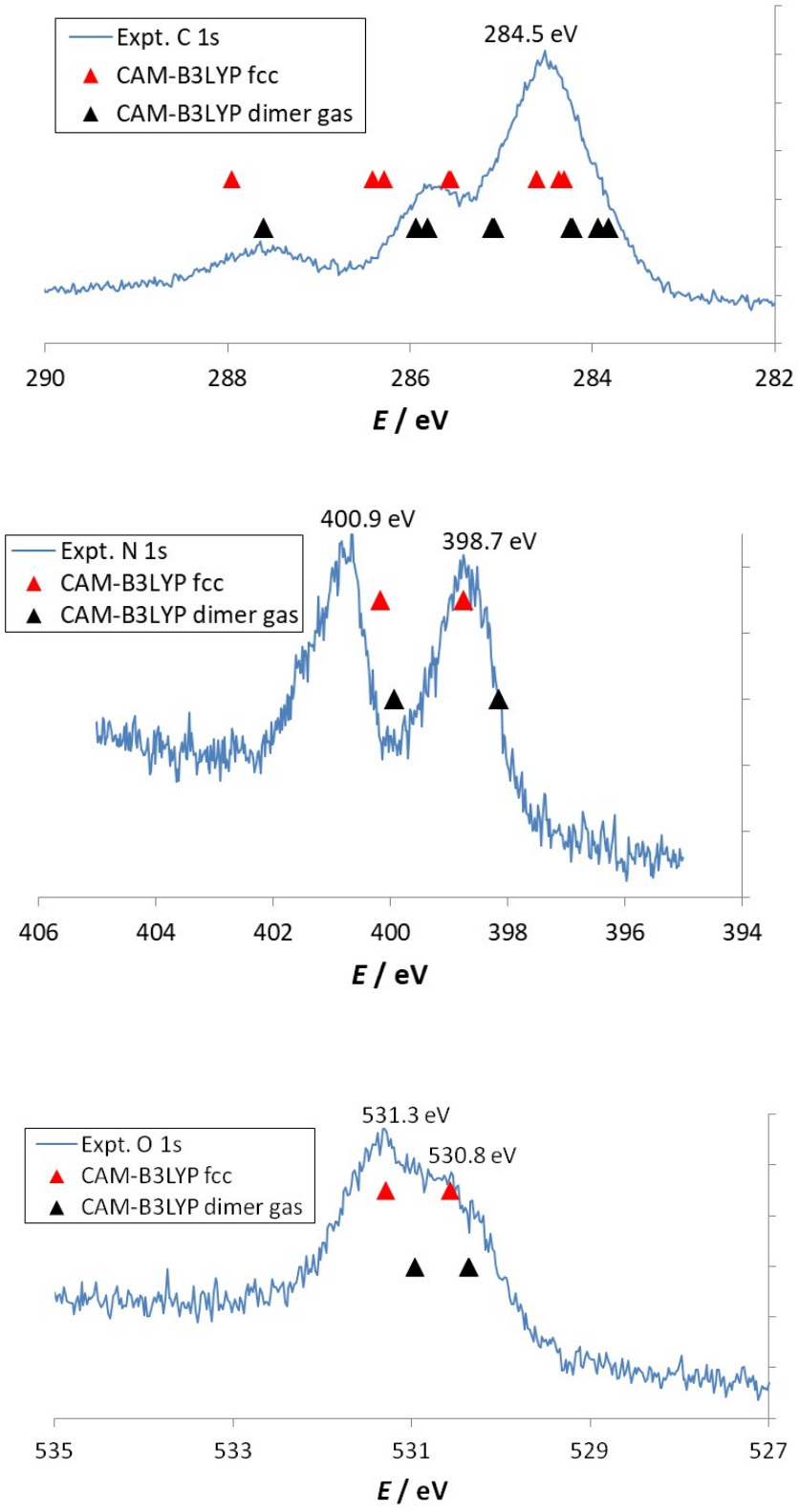


Figure S15. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) XPS spectra of the nit9/Au system (fcc = adsorption via NO on the flat surface above the fcc site). The upward energy shifts of 5.0 (C 1s), 5.4 (N 1s), and 7.5 eV (O 1s) were applied for the modelled spectra.

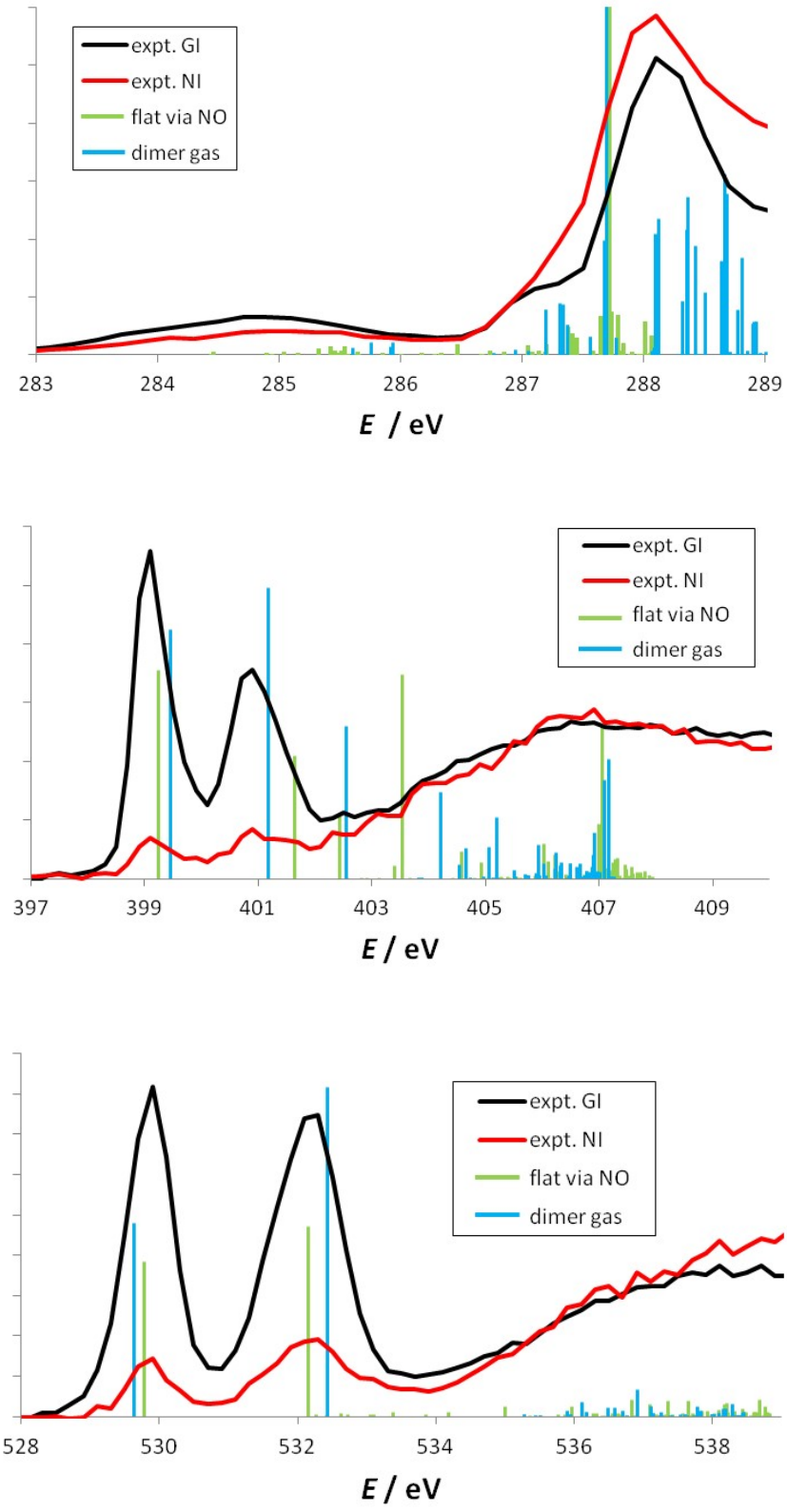


Figure S16. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) NEXAFS spectra of the nit8/Au system (flat via NO = adsorption via NO on the flat surface above the fcc site). The upward energy shifts of 10.2 (C 1s), 12.2 (N 1s), and 13.8 eV (O 1s) were applied for the modelled spectra.

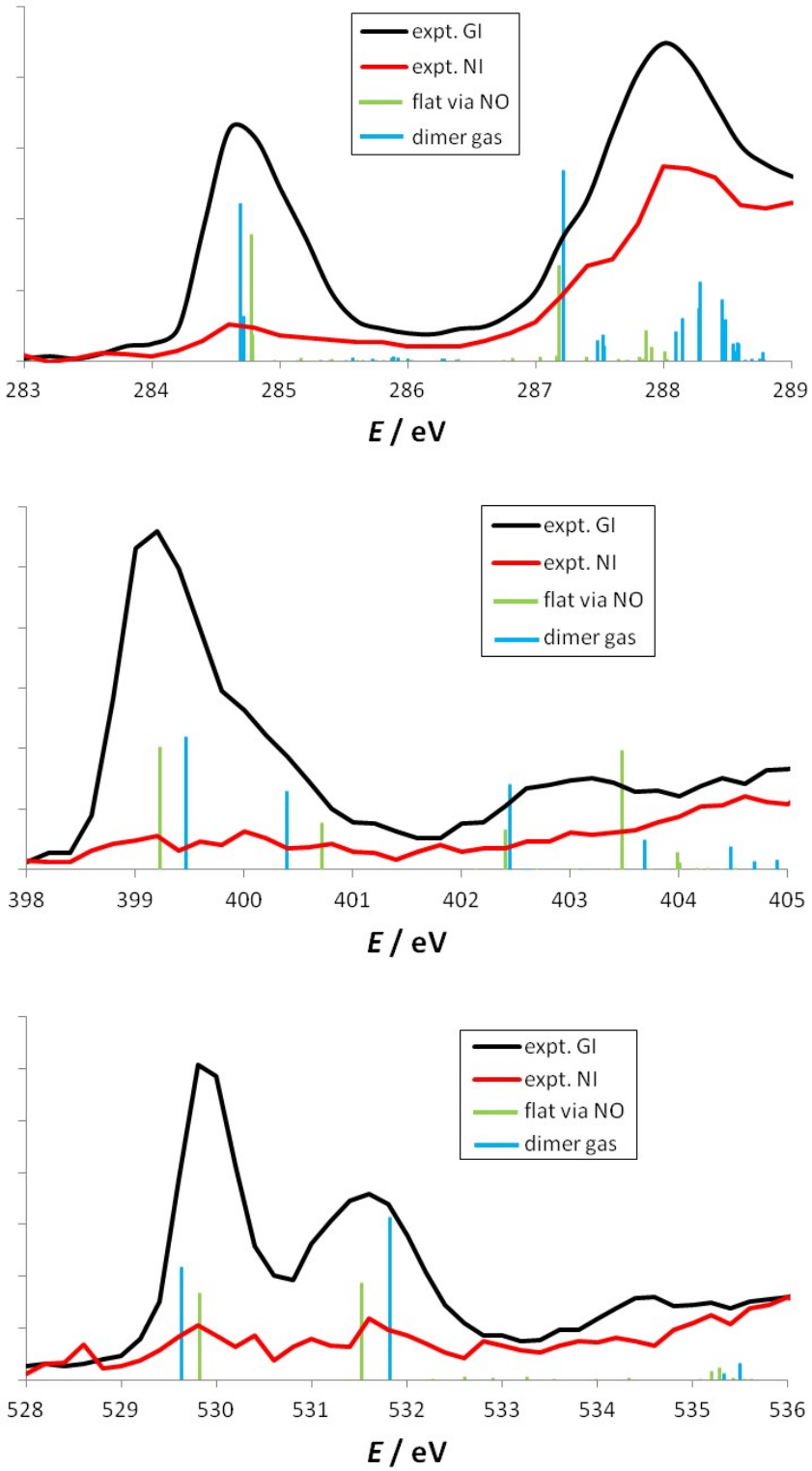
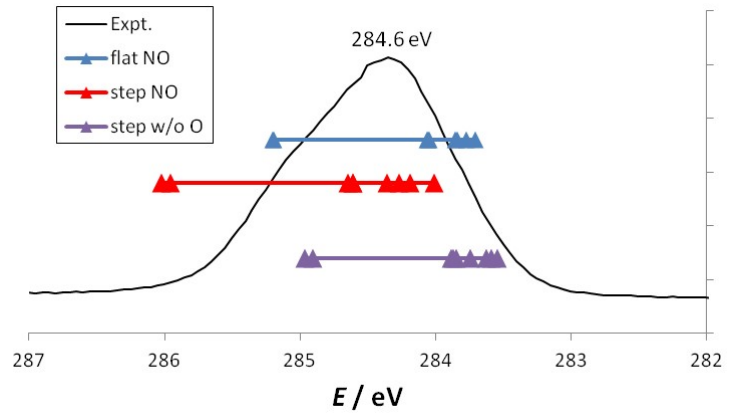
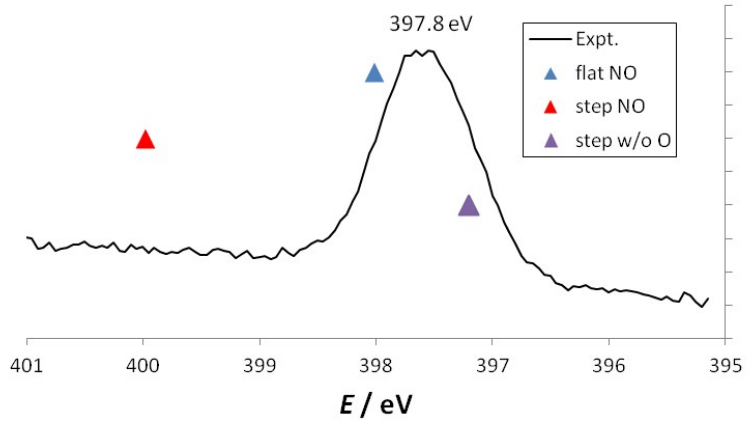


Figure S17. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) NEXAFS spectra of the nit9/Au system (flat via NO = adsorption via NO on the flat surface above the fcc site). The upward energy shifts of 10.2 (C 1s), 12.2 (N 1s), and 13.8 eV (O 1s) were applied for the modelled spectra.





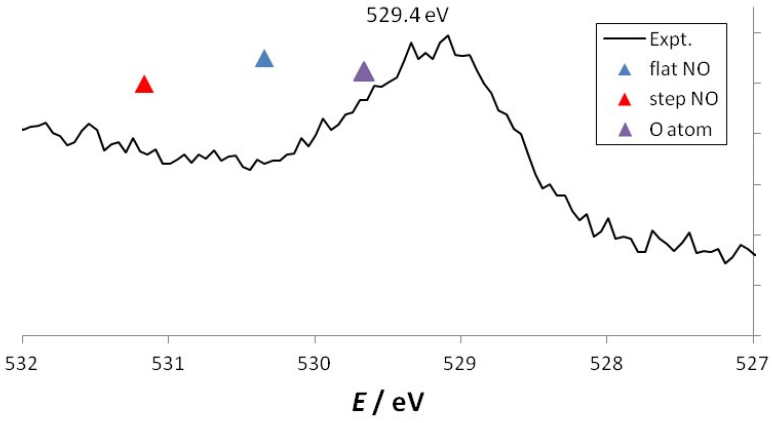


Figure S18. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) XPS spectra of the TEMPO/Cu system. The upward energy shifts of 5.0 (C 1s), 5.4 (N 1s), and 7.5 eV (O 1s) were applied for the modelled spectra.

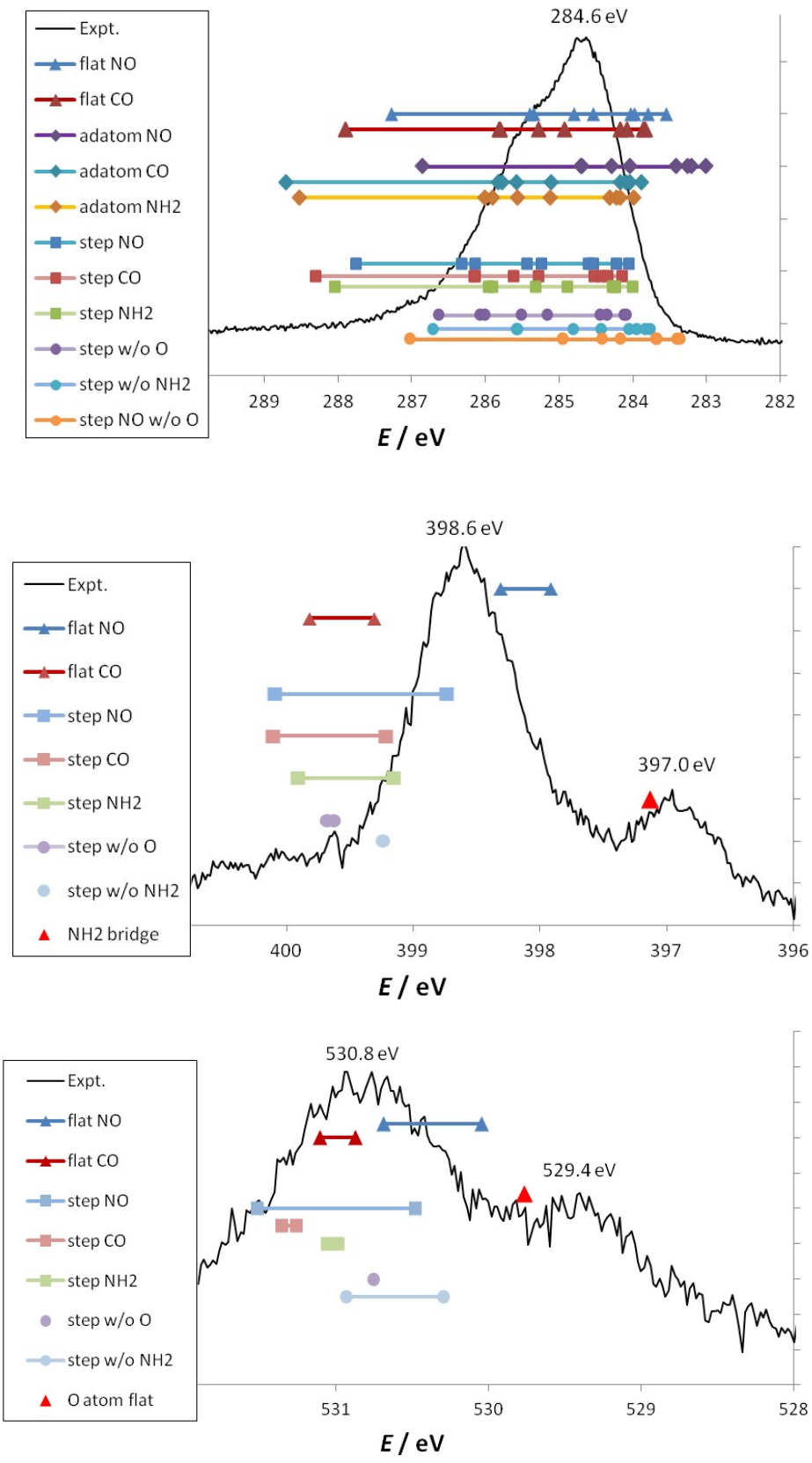


Figure S19. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) XPS spectra of the nit8/Cu system. The upward energy shifts of 5.0 (C 1s), 5.4 (N 1s), and 7.6 eV (O 1s) were applied for the modelled spectra.

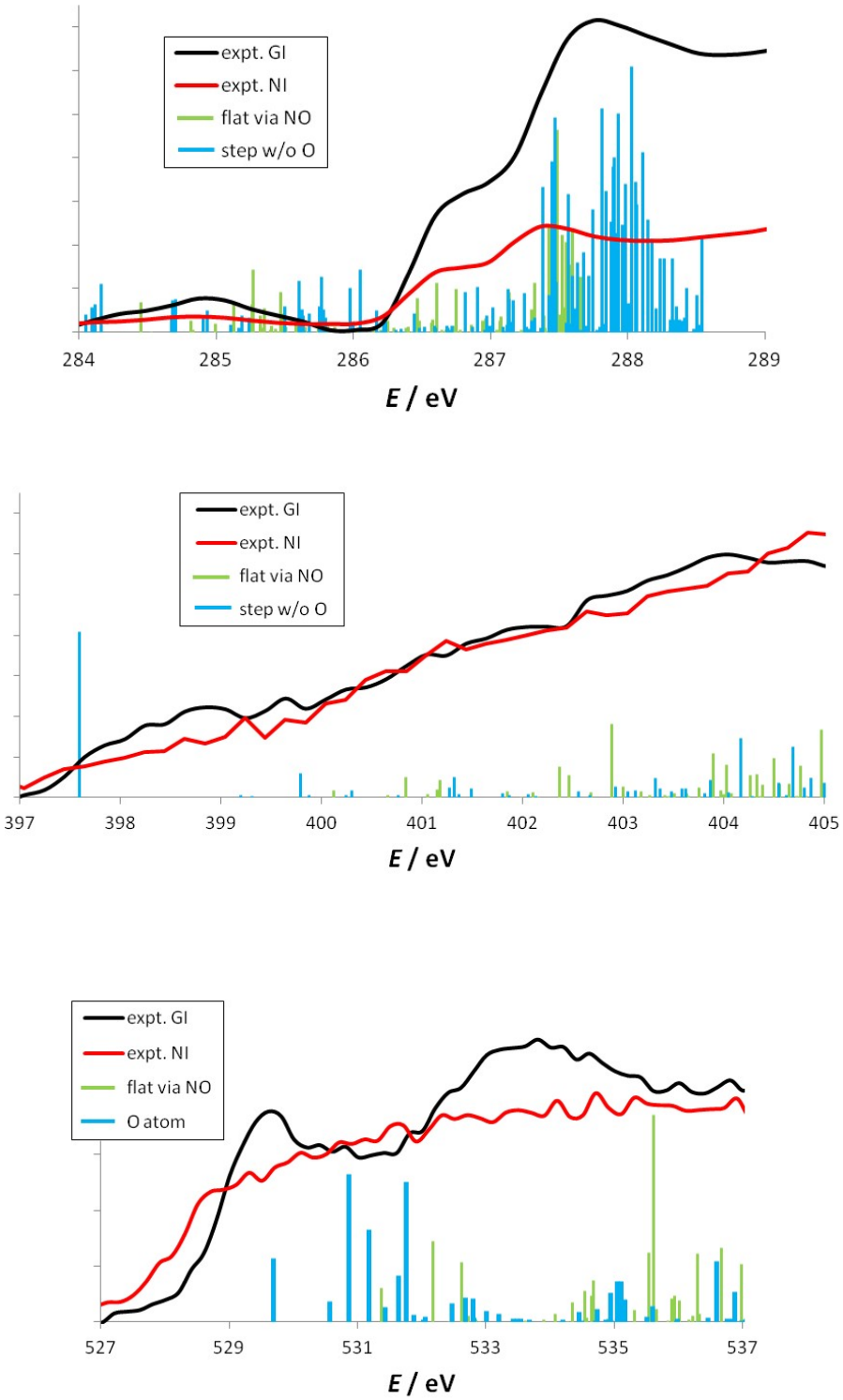


Figure S20. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) NEXAFS spectra of the TEMPO/Cu system. The upward energy shifts of 10.2 (C 1s), 12.2 (N 1s), and 13.8 eV (O 1s) were applied for the modelled spectra.

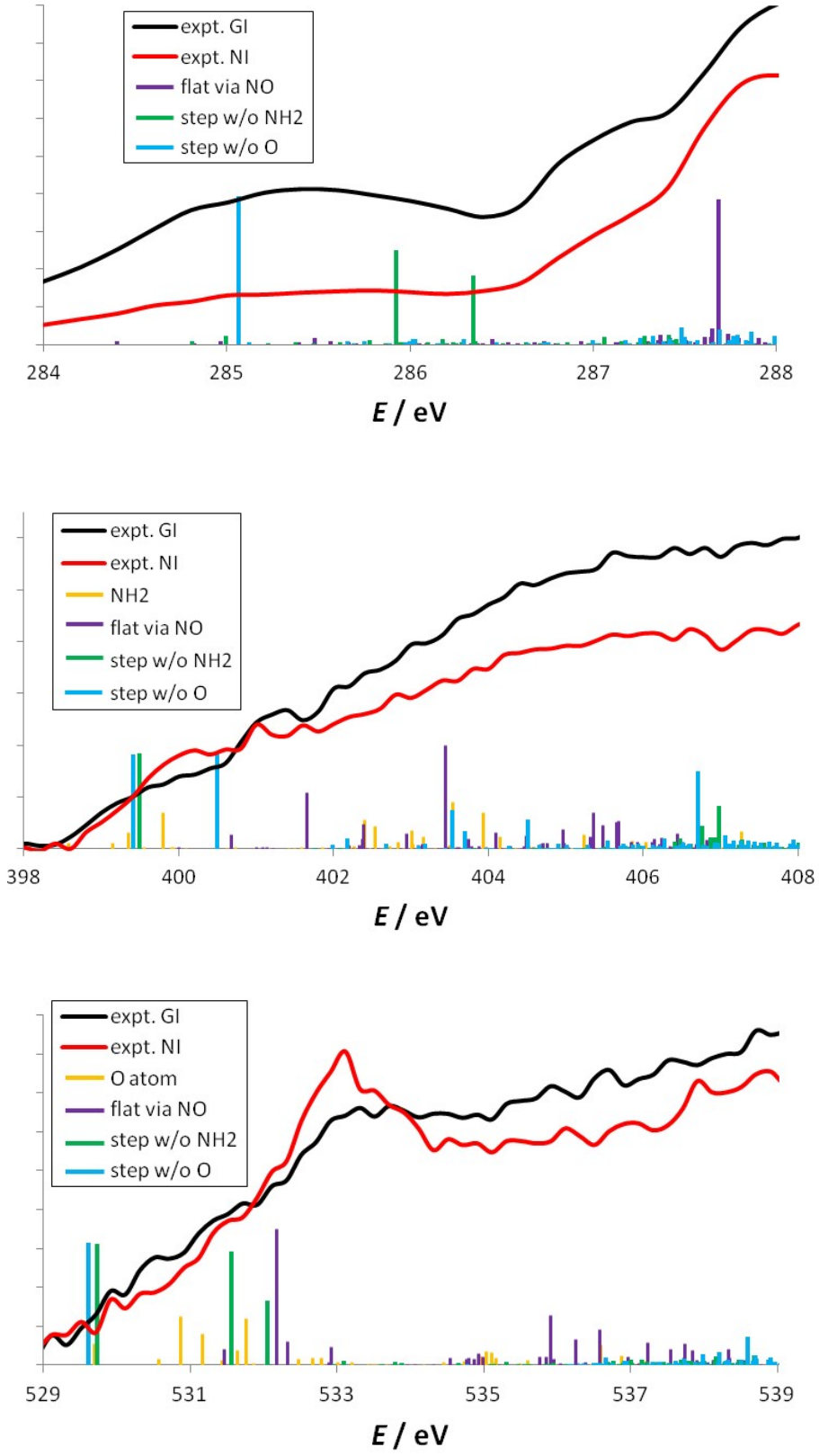


Figure S21. The experimental and modelled (CAM-B3LYP/ ZORA-def2-TZVP) NEXAFS spectra of the nit8/Cu system. The upward energy shifts of 10.2 (C 1s), 12.2 (N 1s), and 13.8 eV (O 1s) were applied for the modelled spectra.

Table S11. The details of computing the reaction energies (page 11 in the manuscript) for the decomposition of the $CONH_2$ anchor on the Cu step atoms are given in the following table (E_{ads} = adsorption energy; E_r = reaction energy; w/o = without). The energies of the C=O and C-NH2 bonds were computed in vacuo at the M06-2X-D3/cc-pVTZ level using the Gaussian 16 suite (Gaussian 16, Revision C.01, M. J. Frisch et al. Gaussian, Inc., Wallingford CT, 2016.)

	eV	kcal mol^{-1}
E_{ads} via CO (on-top step)	–0.97	
E_{ads} nit9 w/o O (on-top step)	–1.99	
E_{ads} O atom (hcp flat)	–5.39	
***E*(C=O bond)**	–6.79	
E_r (C=O scission)	0.38	8.8
E_{ads} via NH_2 (on-top step)	–0.69	
E_{ads} nit9 w/o NH_2 (on-top step)	–1.96	
E_{ads} NH_2 (bridge flat)	–2.72	
***E*(C-NH_2 bond) g16**	–4.30	
E_r (C-NH_2 scission)	0.32	7.3

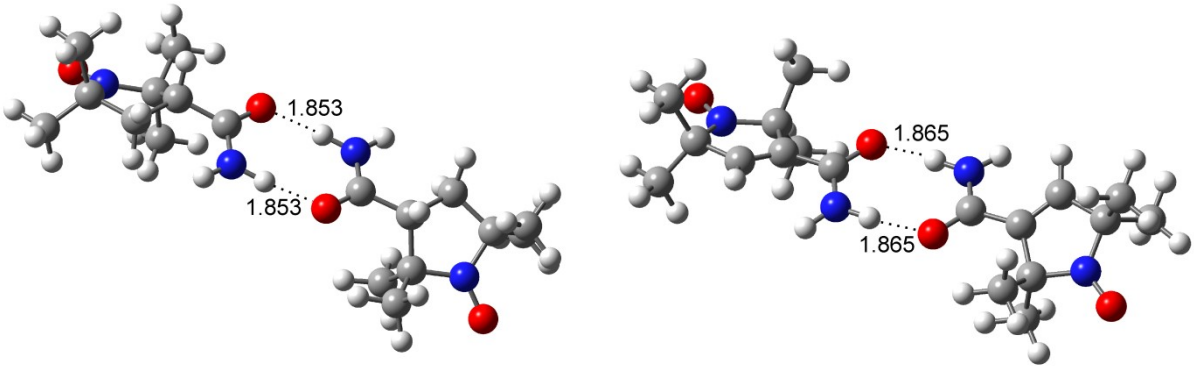


Figure S22. Optimized structures (B3LYP/6-31+G(d,p)) of the hydrogen-bonded dimers of nit8 and nit9. The H-bond lengths are given in Å.

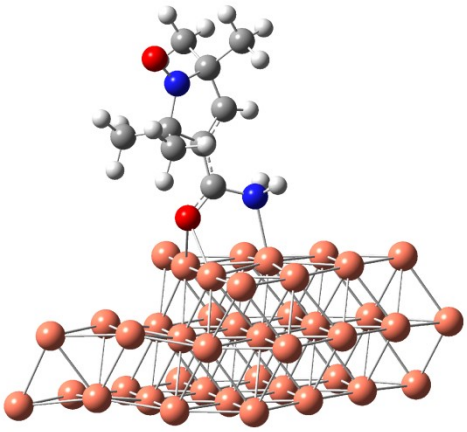


Figure S23. The structure in the nit9/Cu system with both carbonyl and amino group bonded to the Cu step and terrace atoms. The relevant geometric parameters are discussed in the main text. The full Cartesian coordinates and lattice vectors are given below ("Nit9 on Cu step via CO and NH_2").

The Cartesian coordinates and lattice vectors (in Å) for all the structures studied

TEMPO on flat Au(111) hcp site

-0.08633524	0.08067474	-0.21190765	Au
2.82264463	0.07562360	-0.24672167	Au
5.77470870	0.07079518	-0.23054821	Au
1.36851148	2.62121698	-0.25490625	Au
4.29321654	2.61430599	-0.24671109	Au
7.22615837	2.61126783	-0.22843425	Au
2.83231544	5.14328309	-0.24835759	Au
5.75357270	5.13883526	-0.23045555	Au
8.67569353	5.14704090	-0.21666202	Au
1.39055186	0.89253777	-2.74117779	Au
4.31730042	0.89144856	-2.72303461	Au
7.24484346	0.89195666	-2.71380175	Au
2.85579158	3.42345154	-2.75315738	Au
5.77697332	3.42290792	-2.73474066	Au
8.70240167	3.42615748	-2.73046994	Au
4.31691333	5.95488610	-2.75753327	Au
7.24039373	5.95190442	-2.74685191	Au
10.16469560	5.95139727	-2.73579634	Au
-0.04338183	1.70127114	-5.22230759	Au
2.88157874	1.70151093	-5.20937928	Au
5.80450037	1.70191017	-5.19465267	Au
1.42034747	4.23371101	-5.23291816	Au
4.34327887	4.23416100	-5.21826906	Au
7.26610023	4.23369145	-5.20552166	Au
2.88171344	6.76382757	-5.24180042	Au
5.80534972	6.76429778	-5.22992285	Au
8.72922348	6.76511815	-5.21745625	Au
-0.02256693	-0.01162270	-7.71678884	Au
2.90042284	-0.01147103	-7.70074901	Au
5.82708419	-0.01065766	-7.68818437	Au
1.43841525	2.52187132	-7.72824520	Au
4.36403252	2.52198651	-7.71376999	Au
7.28888892	2.52216742	-7.70346847	Au
2.90211127	5.05239367	-7.74211392	Au
5.82557198	5.05266308	-7.73011697	Au
8.74967832	5.05186411	-7.71476797	Au
3.43567347	0.07037654	6.02556777	H
1.76111340	0.67550809	6.17479449	H
3.43191601	2.13758352	7.40260367	H
2.59477894	3.06059159	6.13341604	H
5.08678099	3.50973817	6.05524892	H
5.41154478	1.75644499	5.94170288	H
1.45419970	1.86494575	2.57209922	H
0.45256807	1.19097239	3.89955886	H
1.33590836	2.73507405	4.14799833	H
3.39473979	-1.14112553	3.77861437	H
1.65767035	-1.06210576	4.28342588	H
2.14658671	-0.59994562	2.60760078	H
3.02423933	4.19703311	4.16752856	H
4.64080497	4.80211220	3.67343410	H

```
    3.66905550    3.83970417    2.52063865    H
    6.08943794    2.79631992    2.43580691    H
    6.70710569    3.35649614    4.03421287    H
    6.53750173    1.58708596    3.68485091    H
    3.90040471    1.42577181    3.56815177    N
    2.61576008    0.89196874    4.17589135    C
    2.75688557    0.90616894    5.72907548    C
    3.31597497    2.22576204    6.29700395    C
    4.68042726    2.55126331    5.65648863    C
    4.63932337    2.64208529    4.10052014    C
    1.40049287    1.73135067    3.67740377    C
    2.44796553   -0.56651143    3.67679717    C
    3.94130906    3.94129563    3.59555397    C
    6.07975312    2.58849339    3.52798398    C
    4.17619739    1.05076629    2.35842400    O

outcell: Unit cell vectors (Ang):
        8.772206    0.000845    0.038505
        4.386948    7.593798   -0.037425
        0.140360   -0.221859   26.985405
```

TEMPO on flat Au(111) fcc site

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   -0.13669095    0.06995618   -0.31429845    Au
    2.78442354    0.07787304   -0.28094404    Au
    5.71695966    0.06071531   -0.27525378    Au
    1.32440782    2.60471301   -0.30530822    Au
    4.25107208    2.60786311   -0.27338058    Au
    7.18466134    2.61834340   -0.27004028    Au
    2.80093974    5.12749600   -0.28352289    Au
    5.72193324    5.14740547   -0.26902293    Au
    8.64537651    5.14917207   -0.22304835    Au
    1.35822498    0.89448940   -2.80849045    Au
    4.28354610    0.89963150   -2.76843496    Au
    7.21001139    0.90281391   -2.73303844    Au
    2.82637513    3.42572026   -2.79748378    Au
    5.74828848    3.43264856   -2.76421101    Au
    8.67880783    3.43828582   -2.72977543    Au
    4.29095531    5.95858081   -2.79276007    Au
    7.21699612    5.96469205   -2.75851455    Au
   10.14440118    5.96304750   -2.71967746    Au
   -0.07029340    1.69756259   -5.30382354    Au
    2.85519062    1.70236595   -5.25701518    Au
    5.78017666    1.70808217   -5.22481710    Au
    1.39579680    4.23061019   -5.29502823    Au
    4.32140761    4.23527838   -5.25229803    Au
    7.24532075    4.24053728   -5.21766988    Au
    2.86345256    6.76278023   -5.28772413    Au
    5.78661776    6.76900659   -5.24489079    Au
    8.71297473    6.77465702   -5.20749727    Au
   -0.03635989   -0.01721227   -7.80145294    Au
    2.88574691   -0.01199187   -7.75831155    Au
    5.81277083   -0.00713668   -7.71880601    Au
    1.43002202    2.51750664   -7.79221379    Au
    4.35320950    2.52180455   -7.74868712    Au
    7.28112821    2.52623056   -7.71344719    Au
```

```
    2.89517094    5.04713144   -7.78522844    Au
    5.82070478    5.05616761   -7.74545989    Au
    8.74555678    5.05983631   -7.70698770    Au
    5.08350969    0.63394044    6.09139372    H
    3.39854794    1.20347700    6.26205354   H
    5.04574416    2.68739489    7.49210731   H
    4.18847010    3.60732556    6.23386781   H
    6.67399964    4.09500563    6.15012120   H
    7.02404746    2.34763444    6.02301058   H
    2.99960489    2.40089211    2.68411333   H
    2.05590457    1.75895610    4.07276234   H
    2.95176911    3.30418450    4.24331428   H
    5.01286930   -0.57793240    3.92327012   H
    3.24217923   -0.47955808    4.27926734   H
    3.87613022   -0.01605624    2.65076762   H
    4.64481252    4.81396905    4.30012414   H
    6.24985613    5.39366493    3.74035760   H
    5.22475306    4.42942903    2.63386073   H
    7.69896137    3.43681060    2.53519346   H
    8.31687970    3.91922999    4.15812185   H
    8.11861906    2.16992027    3.73484661   H
    5.49482698    2.02940719    3.64029905   N
    4.22935292    1.46313207    4.25995381   C
    4.38494891    1.45890912    5.81074290   C
    4.92396842    2.78299375    6.38784159   C
    6.28073673    3.13364001    5.74507353   C
    6.23610239    3.23700367    4.19049554   C
    2.99261635    2.28987274    3.79219068   C
    4.08440708    0.00871778    3.74200774   C
    5.53794242    4.54134850    3.69709038   C
    7.67799063    3.18475804    3.61751823   C
    5.71267746    1.73737293    2.39605444   O

outcell: Unit cell vectors (Ang):
        8.775240    0.015291    0.119267
        4.399819    7.598025    0.021589
        0.355930   -0.155341   27.447026
```

TEMPO on flat Au(111) parallel

```
   -0.10992106    0.07992750   -0.81232828     Au
    2.80478789    0.07780714   -0.80830133     Au
    5.73809575    0.07078823   -0.81091077     Au
    1.34149785    2.60777951   -0.83656938     Au
    4.26806065    2.61554712   -0.83956579     Au
    7.18570172    2.61078218   -0.72700470     Au
    2.80464117    5.13697105   -0.81987535     Au
    5.72569115    5.13930413   -0.76739843     Au
    8.64499148    5.13905112   -0.71004443     Au
    1.37930925    0.89532730   -3.33581781     Au
    4.29952129    0.89693381   -3.31290600     Au
    7.22294435    0.89908457   -3.25547531     Au
    2.83803613    3.42805898   -3.34325808     Au
    5.76595533    3.42744512   -3.29664526     Au
    8.67677405    3.42570075   -3.24045183     Au
```

```
     4.29997167    5.95354926   -3.31839490     Au
     7.21818006    5.95208977   -3.27874181     Au
    10.13426195    5.94518092   -3.25087732     Au
    -0.04858939    1.71283033   -5.84052155     Au
     2.86816979    1.71083009   -5.80324556     Au
     5.78867062    1.70957547   -5.76500912     Au
     1.40958314    4.23967838   -5.84238820     Au
     4.32909735    4.23996322   -5.79507325     Au
     7.24699137    4.23972292   -5.74796731     Au
     2.86964955    6.76797122   -5.83355719     Au
     5.78496994    6.76741945   -5.78547029     Au
     8.70300626    6.76675577   -5.75199949     Au
    -0.01505420    0.00432639   -8.34076874     Au
     2.90033525    0.00280719   -8.29740227     Au
     5.82172141    0.00217633   -8.25426123     Au
     1.44266936    2.53422130   -8.34062805     Au
     4.36120630    2.53234656   -8.29527058     Au
     7.27996063    2.53179037   -8.25386837     Au
     2.90314881    5.06129953   -8.33470365     Au
     5.82066876    5.06364550   -8.29074293     Au
     8.73673346    5.05999141   -8.25172920     Au
     4.88417972    4.54916898    5.02242888     H
     4.18568045    5.27396713    3.54607565     H
     6.54728813    4.43274421    3.17042455     H
     5.40012606    3.60426780    2.10115792     H
     6.96426662    1.93142461    3.14969055     H
     6.56627841    2.53919306    4.78395695     H
     1.72373803    2.49788246    2.81456751     H
     1.91699658    4.28362455    2.63123706     H
     3.10410788    3.17748171    1.87986727     H
     2.86080970    3.68418225    6.24962484     H
     2.10964982    4.89702158    5.14456134     H
     1.41772503    3.23384750    5.27570277     H
     4.53236517    1.48673298    1.69524436     H
     5.43981160    0.01302325    2.13701757     H
     3.68293716    0.14456461    2.54187911     H
     4.64026218   -0.63896732    4.82988757     H
     6.37813405   -0.26057636    4.49049206     H
     5.52819866    0.52689477    5.87368872     H
     3.74253202    1.95329525    4.43645162     N
     3.28573544    3.36893719    4.10375946     C
     4.52392793    4.30963454    3.99320470     C
     5.68883826    3.71943196    3.17286261     C
     6.14230267    2.36954780    3.76478977     C
     5.00119198    1.31308048    3.86908522     C
     2.46680327    3.32603993    2.77725425     C
     2.36071936    3.82061030    5.26528265     C
     4.64010022    0.70926655    2.48091461     C
     5.40716152    0.16458211    4.82897114     C
     2.84734373    1.15195050    4.88978905     O

outcell: Unit cell vectors (Ang):
        8.754377   -0.001780    0.130209
        4.374821    7.586114    0.006889
        0.351645   -0.214546   30.303382
```

TEMPO on flat Cu(111) fcc site

-0.03016113	-0.04617272	0.00014950	Cu
2.58190880	-0.01907685	0.08201233	Cu
5.19172242	0.00595413	0.11543118	Cu
7.81317394	0.02116416	0.12921213	Cu
1.30101972	2.22103966	0.05578388	Cu
3.90445139	2.24365910	0.11768418	Cu
6.51301471	2.25701051	0.12890105	Cu
9.13729764	2.27430252	0.11160979	Cu
2.60433618	4.47992118	0.09840723	Cu
5.21614222	4.49845562	0.14027207	Cu
7.83109270	4.51867935	0.16783190	Cu
10.45309510	4.53277010	0.20481081	Cu
3.92718300	6.73909166	0.12131176	Cu
6.53964657	6.74837686	0.18066439	Cu
9.15484863	6.77278499	0.21747977	Cu
11.77226918	6.79642041	0.23777580	Cu
1.30315976	0.75983618	-2.08869819	Cu
3.91138488	0.78474453	-2.03280513	Cu
6.54288282	0.79133083	-2.01786688	Cu
9.16836278	0.80558961	-2.00730897	Cu
2.64662811	3.03086745	-2.07854312	Cu
5.23257763	3.04557440	-2.05763971	Cu
7.82296830	3.05260381	-2.03225936	Cu
10.49388537	3.06168813	-1.95967510	Cu
3.93453963	5.26218593	-2.05227214	Cu
6.51977565	5.25831126	-2.02115122	Cu
9.16529964	5.28073675	-1.93666137	Cu
11.78454995	5.33122827	-1.90865642	Cu
5.24996846	7.48468886	-2.02213077	Cu
7.85071163	7.53983125	-1.92466688	Cu
10.47422614	7.56572027	-1.91003818	Cu
13.10749838	7.59121965	-1.88260192	Cu
0.00995223	1.50536141	-4.28996763	Cu
2.61271962	1.51781164	-4.18524640	Cu
5.23940179	1.49629939	-4.13877416	Cu
7.86618617	1.53368807	-4.17444421	Cu
1.31126028	3.76976478	-4.22792213	Cu
3.90257012	3.77866476	-4.23889886	Cu
6.60213966	3.73646178	-4.24738857	Cu
9.19544691	3.80997311	-4.09994169	Cu
2.61144799	6.04608093	-4.15133185	Cu
5.24011950	6.07104290	-4.21644609	Cu
7.89628776	6.06906939	-4.02715419	Cu
10.48821043	6.07949407	-4.07053234	Cu
3.96479791	8.28553230	-4.17420776	Cu
6.58600739	8.30439419	-4.08730937	Cu
9.19347503	8.31679260	-4.04991453	Cu
11.81688109	8.33141142	-4.06368945	Cu
8.08159245	4.15823959	-7.36055981	H
4.52561361	1.89843227	-7.52484407	H
7.04911736	4.30328655	-9.59216282	H
4.93067138	2.96125383	-9.66718724	H
7.77416861	5.22526457	-7.28217271	C
8.51254293	5.85607311	-7.82680076	H

```
    3.69077210    2.62786291   -7.42822165    C
    6.44821221    5.22476668   -9.40256604    C
    4.34627677    3.89278632   -9.47448078    C
    2.81904608    2.26146802   -8.01650063    H
    7.83717832    5.51503475   -6.20314368    H
    5.24012823    4.89852321  -11.19670190    H
    7.03045098    6.07591813   -9.82441506    H
    5.45426818    4.35981409   -7.27726286    N
    5.09058125    5.07712478  -10.10602683    C
    6.34725396    5.44192402   -7.85563630    C
    3.37548844    2.64827724   -6.35698060    H
    4.12406019    4.03060484   -7.93193003    C
    3.34848342    3.74238057   -9.94777853    H
    5.33660834    4.46962452   -5.84721975    O
    4.49156782    6.01454631  -10.02879677    H
    5.88571314    6.89420430   -7.53860381    C
    3.00036805    5.06398380   -7.62827761    C
    6.69548178    7.61915071   -7.78064301    H
    2.00545903    4.65845953   -7.92157479    H
    5.66533565    7.01101747   -6.44955379    H
    2.95449977    5.27913090   -6.53349285    H
    4.97715570    7.19959514   -8.09865951    H
    3.14047948    6.02966143   -8.15768925    H

outcell: Unit cell vectors (Ang):
       10.465080    0.072750    0.144516
        5.295487    9.028781    0.134356
        0.321090    0.157764   25.577888
```

TEMPO on flat Cu(111) hcp site

```
    0.04808891    0.03181277   -0.00385565     Cu
    2.68889103    0.05654044   -0.01149805     Cu
    5.31204755    0.08026302    0.00177513     Cu
    7.94018728    0.10514852   -0.01770452     Cu
    1.38578833    2.29324261    0.03594079     Cu
    4.02133095    2.31673295    0.01832390     Cu
    6.64516545    2.33491831   -0.00468898     Cu
    9.26943473    2.36677776   -0.01734751     Cu
    2.73521585    4.54294330    0.04983122     Cu
    5.35487479    4.56636254    0.02448881     Cu
    7.97898289    4.58865307    0.00515763     Cu
   10.60191862    4.61979373    0.00305517     Cu
    4.06661911    6.78983031    0.04112096     Cu
    6.69022798    6.81667563    0.00391489     Cu
    9.31992660    6.83970844    0.01388408     Cu
   11.95043234    6.86668627    0.00058182     Cu
    1.36793827    0.77829699   -2.11966980     Cu
    3.99587737    0.80815414   -2.12879479     Cu
    6.62361972    0.79754199   -2.15164012     Cu
    9.24713355    0.84711249   -2.17237047     Cu
    2.68840074    3.02592290   -2.09636839     Cu
    5.33862450    3.05298601   -2.15288006     Cu
    7.90687923    3.05948305   -2.16936252     Cu
   10.55357664    3.09296859   -2.14739753     Cu
```

```
     4.05348461    5.28118830   -2.12668704     Cu
     6.65979595    5.29608814   -2.18038471     Cu
     9.24644280    5.31665716   -2.15507986     Cu
    11.91137469    5.33211837   -2.13040555     Cu
     5.38052180    7.51738065   -2.13420059     Cu
     8.01018605    7.53745553   -2.14728348     Cu
    10.63940639    7.57143073   -2.13963869     Cu
    13.26564625    7.59717160   -2.15771117     Cu
    -0.00463277    1.46028426   -4.28308277     Cu
     2.63029802    1.49448121   -4.27618900     Cu
     5.26272598    1.50368929   -4.27599420     Cu
     7.88986027    1.51945326   -4.32243115     Cu
     1.33669424    3.70466887   -4.23571466     Cu
     3.94884901    3.73481838   -4.21294380     Cu
     6.61896142    3.73629218   -4.37012991     Cu
     9.24520636    3.76629688   -4.26024495     Cu
     2.67011361    5.96328557   -4.21979665     Cu
     5.28606462    6.03566345   -4.33077774     Cu
     7.98686641    6.07253888   -4.33198237     Cu
    10.59033555    6.03375002   -4.24424988     Cu
     4.00334979    8.22981357   -4.26572279     Cu
     6.63468331    8.29187996   -4.22997720     Cu
     9.28894417    8.30477586   -4.25286281     Cu
    11.90109288    8.28905527   -4.31937765     Cu
     9.45266322    4.99354828   -7.52527205     H
     5.87229702    2.72929349   -7.59837167     H
     8.40012106    5.13228787   -9.74091652     H
     6.27410858    3.78020306   -9.76643810     H
     9.15204984    6.06250590   -7.45571883     C
     9.87564425    6.68212507   -8.03231330     H
     5.05133577    3.47419813   -7.49648625     C
     7.79547036    6.05060275   -9.54789135     C
     5.69144404    4.71321859   -9.57721736     C
     4.15844214    3.10642498   -8.05044042     H
     9.24234647    6.37652070   -6.38673433     H
     6.56900853    5.69932517  -11.32076246     H
     8.36783654    6.90263213   -9.98190553     H
     6.82798251    5.19410264   -7.40534589     N
     6.42991117    5.89152335  -10.23112530     C
     7.71415697    6.27297756   -8.00171815     C
     4.77089215    3.51844794   -6.41567540     H
     5.48680917    4.86501154   -8.03341193     C
     4.68910735    4.56091657  -10.03899071     H
     6.73894549    5.28703182   -5.97829764     O
     5.83378192    6.83141465  -10.16089676     H
     7.24996719    7.72264866   -7.67575318     C
     4.36285737    5.90016719   -7.73205792     C
     8.05445073    8.45369602   -7.91696837     H
     3.37174395    5.48793365   -8.02739321     H
     7.03569214    7.82389694   -6.58366597     H
     4.30800642    6.12293162   -6.63913781     H
     6.33742834    8.02720279   -8.22988032     H
     4.50032421    6.86375322   -8.26623596     H

outcell: Unit cell vectors (Ang):
       10.512939    0.104565   -0.052632
```

5.346970	9.014632	-0.000314
-0.132513	0.064119	25.553867

TEMPO on Cu adatom on-top

5.18007130	2.96700283	2.05986370	Cu
0.00523746	-0.13395199	0.14675721	Cu
2.60714394	-0.07767947	0.18714134	Cu
5.20768910	-0.01548117	0.25067215	Cu
7.81531720	0.03078211	0.19341779	Cu
1.34897674	2.16647860	0.11457359	Cu
3.93413853	2.20946581	0.09875658	Cu
6.57329947	2.27083713	0.15093087	Cu
9.16295358	2.32602248	0.16441039	Cu
2.70614846	4.45573045	0.15497423	Cu
5.30685450	4.51678735	0.12303982	Cu
7.90445511	4.56977952	0.19851321	Cu
10.51419542	4.62385400	0.17051804	Cu
4.04654254	6.75737092	0.07059796	Cu
6.65127073	6.81166945	0.13353477	Cu
9.25255820	6.86959005	0.19031871	Cu
11.86167387	6.92189814	0.15087692	Cu
1.25661900	0.65257262	-1.98084817	Cu
3.85744372	0.70813153	-1.96905642	Cu
6.45488081	0.76186556	-1.95223499	Cu
9.06011377	0.81505611	-1.94539841	Cu
2.60349010	2.95471443	-2.02691414	Cu
5.20884415	3.00154992	-2.03706172	Cu
7.80595790	3.06031447	-1.98381636	Cu
10.41557452	3.11719262	-1.95853929	Cu
3.95130418	5.23633768	-2.03296116	Cu
6.55086020	5.29410661	-1.99663416	Cu
9.15363043	5.35787225	-1.93638497	Cu
11.77451557	5.40784150	-1.95190595	Cu
5.30088387	7.53704761	-2.04211959	Cu
7.90235655	7.59655961	-1.98719025	Cu
10.50073185	7.65716960	-1.95769776	Cu
13.10731988	7.70193155	-2.00148181	Cu
-0.05093957	1.34947466	-4.15034207	Cu
2.54718049	1.40329281	-4.13710118	Cu
5.15317563	1.45537747	-4.11955278	Cu
7.76078768	1.50835115	-4.10019355	Cu
1.29519235	3.65112690	-4.17685591	Cu
3.89832853	3.70383794	-4.16430340	Cu
6.50619557	3.75934088	-4.13988289	Cu
9.11355634	3.81265510	-4.08121757	Cu
2.64160490	5.94503118	-4.19776647	Cu
5.24872038	6.00132533	-4.17275513	Cu
7.85849551	6.05217155	-4.09720975	Cu
10.45522078	6.10914385	-4.07588016	Cu
3.99246134	8.23771440	-4.21770993	Cu
6.59619093	8.29406535	-4.14627918	Cu
9.20157606	8.34382595	-4.12722372	Cu
11.80136563	8.40057897	-4.13062647	Cu
6.13988993	0.60454452	5.58531706	H

```
    5.15221986    1.38418233    7.62065767     H
    5.12132459    0.45418684    5.16047799     C
    6.45437177    4.79596027    5.89419229     H
    4.76800155   -0.56081099    5.44686528     H
    5.20038372    0.49333411    4.05240220     H
    5.34981214    3.90052813    7.80192950     H
    4.10716542    1.50504347    7.24619034     C
    5.47970739    5.17172430    5.50991770     C
    4.13472225    1.53667430    5.68591732     C
    4.68737814    2.87142317    5.23123785     N
    3.55126611    0.59384207    7.56517109     H
    4.75283980    2.98484723    3.89187595     O
    4.30098754    4.00314232    7.43268417     C
    5.56160025    5.27400136    4.40702665     H
    3.53925952    2.68570085    8.99933397     H
    3.50161556    2.76884361    7.88778445     C
    5.28916638    6.17647343    5.94784258     H
    4.33303754    4.19212164    5.88650167     C
    3.89461166    4.93410938    7.89111678     H
    2.71844322    1.28906840    5.08043683     C
    2.40735490    0.23323668    5.24280433     H
    2.73506733    1.48073711    3.98464477     H
    2.42154025    2.87388532    7.62837478     H
    2.97739367    4.74202981    5.33984072     C
    1.94147253    1.94172161    5.53351284     H
    2.95110702    4.64289475    4.23231326     H
    2.86562545    5.81960752    5.59468943     H
    2.09445946    4.21086122    5.75693029     H

outcell: Unit cell vectors (Ang):
       10.412794    0.218517    0.072872
        5.393522    9.189657   -0.097999
        0.205970   -0.438325   29.897925
```

TEMPO on Cu step on-top

```
    7.97750477    0.10483175   -0.16560228     Cu
    6.64403666    2.34624193    0.03300069     Cu
    9.26946325    2.35529651   -0.20472309     Cu
    5.36374478    4.61628897   -0.14965713     Cu
    7.95759435    4.61821013   -0.12370358     Cu
   10.51622539    4.60246989   -0.26157514     Cu
    4.07716365    6.82137385   -0.12581913     Cu
    6.65450488    6.84045475   -0.19400191     Cu
    9.23648933    6.83658197   -0.25796567     Cu
   11.82120384    6.80355832   -0.32696222     Cu
    1.44475348    0.82074914   -1.83409389     Cu
    4.02546718    0.81911707   -1.89604449     Cu
    6.57702431    0.83477443   -2.14462624     Cu
    9.19931185    0.82605165   -2.27202597     Cu
    2.74387825    3.06256712   -1.90358350     Cu
    5.28521748    3.02874787   -2.11477282     Cu
    7.87367562    3.05385128   -2.23756324     Cu
   10.51219618    3.03996826   -2.30213110     Cu
    4.00611303    5.27978420   -2.20568935     Cu
    6.60009386    5.29997956   -2.29467616     Cu
```

```
     9.17838563    5.29752890   -2.36170204     Cu
    11.77184343    5.27717507   -2.39783665     Cu
     5.31475467    7.54967674   -2.26587328     Cu
     7.89017683    7.57267134   -2.31102604     Cu
    10.46402819    7.54946943   -2.38903917     Cu
    13.04093525    7.52922448   -2.46814562     Cu
     0.13918467    1.54411389   -4.20083029     Cu
     2.70230284    1.54498404   -4.04905063     Cu
     5.26181982    1.54443567   -4.26653608     Cu
     7.84590928    1.55076420   -4.41069938     Cu
     1.42954852    3.76828715   -4.26068212     Cu
     3.97923244    3.76721983   -4.29212755     Cu
     6.55687297    3.77603450   -4.39523330     Cu
     9.14388020    3.77567674   -4.47126916     Cu
     2.69938248    6.01363172   -4.38792758     Cu
     5.26801595    6.01441241   -4.44065820     Cu
     7.85015444    6.01544491   -4.49683442     Cu
    10.42803518    6.01106518   -4.56556365     Cu
     3.98099706    8.24694059   -4.42834502     Cu
     6.55994925    8.25644646   -4.43442344     Cu
     9.13360357    8.25827281   -4.49377927     Cu
    11.71341141    8.25121461   -4.58794136     Cu
     7.17111647    1.04667011    5.78520579     H
     6.27048418   -0.43415949    5.35379294     H
     4.81624134    1.25399085    6.56634197     H
     4.18327809    0.95863387    4.92952099     H
     4.28373992    3.45522629    5.43059085     H
     6.02007063    3.30242127    5.82201141     H
     6.11214244    0.18122229    1.63836016     H
     6.16272896   -1.15195640    2.83724150     H
     4.81983585    0.04512146    2.88354717     H
     8.92026585    1.01400105    4.17965488     H
     8.42298681   -0.66203143    3.71933097     H
     8.62964270    0.60401405    2.44917986     H
     3.74576243    2.10018129    2.96534769     H
     3.62542250    3.89301499    2.87618091     H
     4.63767393    3.00215425    1.68788205     H
     6.43115405    4.85941628    2.52277041     H
     5.33171751    5.37473780    3.85983572     H
     6.99830627    4.78307048    4.23082555     H
     6.67748113    2.26745548    3.23554492     N
     6.78456952    0.81238806    3.64159744     C
     6.35427295    0.65490129    5.13283186     C
     5.04846949    1.39188589    5.48444662     C
     5.20993388    2.89137140    5.17298739     C
     5.56337495    3.19280460    3.68328019     C
     5.91040294   -0.07544407    2.70641073     C
     8.28066622    0.41773306    3.49017076     C
     4.31858632    3.02999899    2.76063808     C
     6.11570619    4.64046247    3.56737005     C
     7.24036118    2.57606647    2.05742518     O

outcell: Unit cell vectors (Ang):
       10.301973    0.001464   -0.241385
        5.151897    8.920851   -0.177821
       -0.628144   -0.171407   29.282047
```

TEMPO w/o O on Cu step on-top

7.96056890	0.10348941	-0.13353415	Cu
6.66805314	2.35705105	0.21652544	Cu
9.25581939	2.33651156	-0.21356850	Cu
5.37869127	4.59212333	-0.06227328	Cu
7.95737887	4.60222328	-0.14311467	Cu
10.53563686	4.57405515	-0.26444250	Cu
4.08118504	6.82127708	-0.11234499	Cu
6.65405570	6.82523734	-0.18041153	Cu
9.23975225	6.77007780	-0.26621852	Cu
11.82522167	6.79939934	-0.28669071	Cu
1.43028663	0.80403449	-1.97107250	Cu
3.99178159	0.80713314	-2.18643630	Cu
6.56059151	0.82146768	-2.14441549	Cu
9.18185718	0.81022839	-2.26284778	Cu
2.71921280	3.04195462	-2.02775559	Cu
5.27595198	3.01950720	-2.09588014	Cu
7.83401608	3.02458503	-2.19804766	Cu
10.49756820	3.03034897	-2.31045211	Cu
3.99962255	5.26321149	-2.16553801	Cu
6.57647979	5.28174202	-2.26933549	Cu
9.16784241	5.27873503	-2.36420780	Cu
11.76437419	5.27881591	-2.39183980	Cu
5.30685513	7.54172856	-2.24467849	Cu
7.88395785	7.55093792	-2.30842176	Cu
10.45815905	7.53820234	-2.38830351	Cu
13.03869057	7.53716261	-2.39489136	Cu
0.10239167	1.52770024	-4.27340466	Cu
2.65950125	1.54376662	-4.24135363	Cu
5.25573269	1.53813557	-4.33908518	Cu
7.82895847	1.53718124	-4.40545323	Cu
1.39361968	3.76447314	-4.35178538	Cu
3.96326723	3.76383867	-4.28719881	Cu
6.54274985	3.76630076	-4.37890125	Cu
9.12021924	3.76420467	-4.44555100	Cu
2.69106118	6.00513781	-4.39407728	Cu
5.25031480	6.00591004	-4.42214120	Cu
7.83211957	6.00623765	-4.48842337	Cu
10.41093208	6.00493275	-4.56908541	Cu
3.96894967	8.23795753	-4.41395154	Cu
6.54264310	8.24503064	-4.41960497	Cu
9.12258152	8.24599305	-4.52740615	Cu
11.71219729	8.24900866	-4.54408901	Cu
5.32001841	-0.28424095	3.25025727	H
3.63140349	0.16482243	3.62948410	H
5.21758002	0.53260297	5.59596423	H
4.46882356	2.06702785	5.09445560	H
6.97244211	2.36454195	5.37843723	H
7.26603840	0.98741163	4.27646959	H
3.49432584	3.24891234	1.46022100	H
2.46970224	1.94977067	2.16700296	H
3.36042239	3.07359776	3.24800088	H
5.25811285	-0.10381867	0.87897230	H
3.45463020	0.06369768	1.05613585	H
4.37997443	1.23126874	0.05995679	H

```
    5.02881019    4.12117304    4.13856052     H
    6.69495503    4.71762896    4.39570906     H
    5.93184655    4.86506919    2.76739308     H
    8.26989427    3.77649795    2.10394005     H
    8.67860840    3.43496041    3.82173102     H
    8.61086168    2.08335976    2.61893471     H
    5.96323545    2.21839577    2.04491529     N
    4.64450573    1.52719608    2.23246312     C
    4.65521921    0.58258870    3.48353216     C
    5.17080530    1.26766738    4.75789081     C
    6.57223550    1.83794105    4.48036013     C
    6.62908496    2.81751259    3.25073731     C
    3.42603034    2.51008055    2.29372209     C
    4.41898440    0.62510593    1.00086320     C
    6.02859009    4.20651146    3.66233968     C
    8.13194500    3.03947714    2.93505215     C

outcell: Unit cell vectors (Ang):
       10.308650    0.009834   -0.174446
        5.163324    8.933236   -0.092569
       -0.420100    0.002844   30.065148
```

Nit8 on flat Au(111) via NO hcp site

```
   -0.08663957    0.08643552   -0.35109099     Au
    2.81532287    0.07805639   -0.41212543     Au
    5.78745533    0.07243964   -0.38952842     Au
    1.36563616    2.62152702   -0.40536979     Au
    4.29194264    2.62007376   -0.39897456     Au
    7.22601470    2.61145428   -0.36391848     Au
    2.83393654    5.14057418   -0.38144238     Au
    5.75427367    5.13073001   -0.37013280     Au
    8.67934858    5.13941585   -0.36841268     Au
    1.39047990    0.89818974   -2.89452645     Au
    4.32125092    0.89596716   -2.87094047     Au
    7.25198359    0.89475719   -2.85348067     Au
    2.85562159    3.42701654   -2.90150561     Au
    5.78189106    3.42299343   -2.88265857     Au
    8.70662017    3.42220756   -2.87053347     Au
    4.31717183    5.95176691   -2.90150360     Au
    7.24192734    5.94574423   -2.89589090     Au
   10.17082644    5.94296468   -2.87403827     Au
   -0.03260217    1.70098407   -5.37778162     Au
    2.89414304    1.69867394   -5.35746456     Au
    5.81733540    1.69643839   -5.33799369     Au
    1.42958199    4.22894502   -5.38729017     Au
    4.35384829    4.22731196   -5.36414669     Au
    7.27798849    4.22505463   -5.35044592     Au
    2.89006935    6.75395960   -5.39426214     Au
    5.81445490    6.75214499   -5.37656883     Au
    8.74091987    6.75231626   -5.36137549     Au
   -0.00361755   -0.01574647   -7.86925618     Au
    2.91891248   -0.01822773   -7.84783109     Au
    5.84948341   -0.01940926   -7.82791624     Au
    1.45468687    2.51354065   -7.87927621     Au
```

```
    4.38250997    2.51259968   -7.86161322     Au
    7.30787332    2.50874911   -7.84171124     Au
    2.91901666    5.03934363   -7.89484600     Au
    5.84166070    5.03790394   -7.87596353     Au
    8.77022448    5.03429841   -7.85362808     Au
    4.31261350    0.70649338    2.08994203     O
    6.10355806   -0.62896997    4.81197856     H
    3.10375404   -1.72433486    3.79474170     H
    6.76634277    0.08959476    3.29860860     H
    6.41963055    0.32421294    4.33060640     C
    7.26227894    0.75212887    4.91503833     H
    3.66207361   -0.51006723    5.83865915     H
    2.35408746   -0.92821110    3.58720528     C
    4.05324170    0.36557605    7.98929701     H
    5.49933414    0.94124661    8.80419486     H
    4.93826986    0.87003485    7.95324458     N
    1.40914985   -1.18149997    4.11833245     H
    2.14939011   -0.92816914    2.49306539     H
    3.30130573    0.50093535    5.53686556     C
    5.36924065    1.57272938    6.84267712     C
    5.25254848    1.34850316    4.24975281     C
    2.86702962    0.45808872    4.04321793     C
    4.17865294    0.75898207    3.36941069     N
    6.42447984    2.22652986    6.85606209     O
    4.45742442    1.53777491    5.59376186     C
    2.44887353    0.77157178    6.19974149     H
    5.75000262    2.68673898    3.64883742     C
    6.29424843    2.51048829    2.69419168     H
    6.42541314    3.18188447    4.38065793     H
    1.84729573    1.56748214    3.65965795     C
    4.01052925    2.56107347    5.56556919     H
    0.84681474    1.35218316    4.09628339     H
    1.74301717    1.60981516    2.55134425     H
    4.89919778    3.36830717    3.42166456     H
    2.17121881    2.57307176    4.00911643     H

outcell: Unit cell vectors (Ang):
        8.776990   -0.005989    0.057851
        4.383106    7.580767   -0.035625
        0.182817   -0.243560   27.714439
```

Nit8 on flat Au(111) via NO fcc site

```
   -0.09566388    0.07892384   -0.31626519     Au
    2.81774612    0.08511260   -0.30910205     Au
    5.75379750    0.04889204   -0.32936204     Au
    1.35944082    2.61233103   -0.29984502     Au
    4.27624985    2.62230576   -0.34254087     Au
    7.23081256    2.62149004   -0.33024053     Au
    2.82792899    5.13194666   -0.29861701     Au
    5.75213931    5.14394675   -0.28882987     Au
    8.67095381    5.13978301   -0.26139719     Au
    1.38405775    0.89685200   -2.82504484     Au
    4.30985296    0.89644954   -2.80537214     Au
    7.23733405    0.89267385   -2.77983076     Au
```

```
     2.84279317    3.42520367   -2.83177165     Au
     5.77251387    3.42512551   -2.80837136     Au
     8.70191122    3.42563494   -2.78828050     Au
     4.31065730    5.95005193   -2.82441291     Au
     7.23463675    5.95000884   -2.80924705     Au
    10.16006085    5.94204028   -2.78993341     Au
    -0.04889029    1.69462948   -5.31739786     Au
     2.87750100    1.69465873   -5.29143094     Au
     5.80143779    1.69564362   -5.27282599     Au
     1.41407183    4.22369182   -5.32204363     Au
     4.33967076    4.22593280   -5.29256301     Au
     7.26155351    4.22491224   -5.27376370     Au
     2.87700969    6.75201991   -5.32337364     Au
     5.80050746    6.75183737   -5.29482779     Au
     8.72519975    6.75372402   -5.27691897     Au
    -0.02285304   -0.02649565   -7.81358289     Au
     2.89635222   -0.02608143   -7.79045451     Au
     5.82455850   -0.02659687   -7.76252260     Au
     1.43658044    2.50493540   -7.82118844     Au
     4.35894945    2.50624126   -7.79488127     Au
     7.28733605    2.50491672   -7.77162872     Au
     2.89844692    5.03172718   -7.82695599     Au
     5.82308902    5.03500074   -7.80583495     Au
     8.74883461    5.03207405   -7.78008634     Au
     5.75319755    1.60169117    2.07993701     O
     7.53881082    0.20492833    4.78681727     H
     4.57055389   -0.89345174    3.78516132     H
     8.21767347    0.95524326    3.29471075     H
     7.85815597    1.16768543    4.32724743     C
     8.69291728    1.58668400    4.92947855     H
     5.11767803    0.31922515    5.82381662     H
     3.82368020   -0.09976309    3.55914576     C
     5.50671064    1.18317532    7.98404322     H
     6.95599036    1.75653696    8.79127907     H
     6.39965151    1.67300605    7.93800256     N
     2.86461743   -0.35942584    4.06101349     H
     3.65042721   -0.09935055    2.45833220     H
     4.74742714    1.32757849    5.52556536     C
     6.80302813    2.41269446    6.84055924     C
     6.69465521    2.19575708    4.24936898     C
     4.31457000    1.28941214    4.03056831     C
     5.62150629    1.61995114    3.36071855     N
     7.84225376    3.09162671    6.86050968     O
     5.89289331    2.37517486    5.59071257     C
     3.89157628    1.58654987    6.18853243     H
     7.20502573    3.53538445    3.66254981     C
     7.79247002    3.36414142    2.73290753     H
     7.84668086    4.03626951    4.42005059     H
     3.27594047    2.38510399    3.65828133     C
     5.43781276    3.39470027    5.56231946     H
     2.28785692    2.16267300    4.11883544     H
     3.14424174    2.41926432    2.55260974     H
     6.35756107    4.20724046    3.39866193     H
     3.59708563    3.39649146    3.99294482     H

outcell: Unit cell vectors (Ang):
```

8.774221	0.000277	0.073377
4.386947	7.584975	-0.019113
0.234116	-0.218594	27.368179

Nit8 on flat Au(111) via >CO

-0.12152281	0.05302079	-0.50543753	Au
2.79267601	0.05804274	-0.47976924	Au
5.71210892	0.04862137	-0.51546744	Au
1.33520605	2.59014088	-0.50468789	Au
4.22954888	2.59942714	-0.59022983	Au
7.20257653	2.59587450	-0.57271078	Au
2.78610353	5.11919837	-0.49064767	Au
5.71222367	5.11381732	-0.52471198	Au
8.63739600	5.11887892	-0.45560491	Au
1.36730106	0.87535178	-3.01767517	Au
4.28429951	0.87046257	-3.02569717	Au
7.20853112	0.86747709	-2.99527876	Au
2.81263419	3.41041257	-3.06013237	Au
5.74451249	3.40271343	-3.04207522	Au
8.67292172	3.40409680	-3.00557472	Au
4.27993754	5.92743997	-3.04195031	Au
7.20617848	5.92642755	-3.02004459	Au
10.12657724	5.91993979	-3.00635056	Au
-0.05472121	1.68533207	-5.51909957	Au
2.86516123	1.68429196	-5.50874400	Au
5.78890290	1.68348503	-5.49929221	Au
1.40136005	4.21545341	-5.53872725	Au
4.32435492	4.21324436	-5.52259701	Au
7.24565583	4.21111950	-5.49687999	Au
2.86349654	6.74019945	-5.53879428	Au
5.78447010	6.73909117	-5.50877580	Au
8.70369914	6.73634450	-5.50044067	Au
-0.02048923	-0.02316398	-8.02442508	Au
2.89732375	-0.02529707	-8.01024822	Au
5.82102650	-0.02916240	-7.98870438	Au
1.43657655	2.50602418	-8.03857573	Au
4.35487363	2.50354197	-8.02209518	Au
7.28238233	2.50148956	-7.99583352	Au
2.89319902	5.03099425	-8.05016830	Au
5.81637623	5.03528972	-8.02772880	Au
8.73726487	5.02764116	-8.00884870	Au
8.61030675	3.37475702	6.04183616	H
8.38567658	2.61176869	7.65993952	H
7.96042098	3.35170197	6.94524722	C
7.99252927	4.35996584	7.41486190	H
7.60508251	2.49249998	4.03219025	H
7.63820798	4.91571943	3.75668551	H
7.10032275	0.98413575	5.91046793	H
6.59293215	4.79221135	3.39120799	C
6.51838946	2.32319250	4.22723841	C
6.48576249	3.00723674	6.59086158	C
6.62646850	4.47499236	2.32539228	H
6.34950463	1.76844185	5.66542994	C
6.07240776	1.43369646	3.05271995	C

```
    5.97615905    1.92294635    1.90939712     O
    5.81516811    0.10666113    3.29085824     N
    5.93474535    4.09110000    5.70132889     N
    5.83037018    3.73937432    4.23487516     C
    5.90840518   -0.31523020    4.21423935     H
    6.09083622    5.78279628    3.45982460     H
    6.00643550    2.10084895    8.53859959     H
    5.73551066    5.28865156    6.13136813     O
    5.63257103    2.91423387    7.87699926     C
    5.59410932   -0.48639279    2.48142594     H
    5.68145287    3.87710592    8.43062769     H
    5.33487642    1.32471439    5.79431099     H
    4.32500193    3.72698930    3.84312582     C
    4.56576205    2.71028316    7.63493552     H
    4.19453363    3.56572588    2.75023852     H
    3.88328788    4.71288950    4.11417246     H
    3.76165624    2.93636693    4.38888504     H

outcell: Unit cell vectors (Ang):
        8.763916   -0.005131    0.060449
        4.377041    7.578661   -0.025998
        0.182292   -0.225826   28.492356
```

Nit8 on flat Au(111) parallel

```
   -0.09363375    0.07280035   -0.42694737     Au
    2.82929663    0.06400278   -0.43321538     Au
    5.75672364    0.07092932   -0.35791599     Au
    1.35536263    2.60977746   -0.58027502     Au
    4.29046850    2.59700726   -0.45913067     Au
    7.21675750    2.59613195   -0.38371088     Au
    2.82447988    5.12814162   -0.43725038     Au
    5.74790499    5.11337771   -0.37485440     Au
    8.67226613    5.12374320   -0.36709426     Au
    1.39279191    0.87907406   -2.97776250     Au
    4.32133659    0.88109378   -2.92558579     Au
    7.24551507    0.88083544   -2.86388679     Au
    2.85901508    3.41933117   -2.99553051     Au
    5.78104616    3.41048455   -2.92735713     Au
    8.69519394    3.41514294   -2.92118531     Au
    4.31795498    5.93096951   -2.95334301     Au
    7.23630400    5.92166238   -2.93304085     Au
   10.16675234    5.92975196   -2.88688986     Au
   -0.05008596    1.68598396   -5.46896061     Au
    2.88222648    1.68782438   -5.43815907     Au
    5.80768227    1.68623618   -5.38684204     Au
    1.41509436    4.21660381   -5.48169708     Au
    4.34422972    4.21345612   -5.43880677     Au
    7.26620867    4.20976201   -5.40897077     Au
    2.87619180    6.73524925   -5.46729012     Au
    5.80238871    6.73376113   -5.44575055     Au
    8.72982716    6.73182112   -5.40671807     Au
   -0.02285861   -0.02481536   -7.95588634     Au
    2.90821868   -0.02489536   -7.92103044     Au
    5.83513830   -0.02524991   -7.88557892     Au
    1.44192048    2.50139992   -7.97054665     Au
```

```
    4.36951394    2.50001373   -7.93566565     Au
    7.29421276    2.49814055   -7.90346030     Au
    2.90484757    5.02589562   -7.97980838     Au
    5.82991441    5.02368234   -7.94127294     Au
    8.75502837    5.02333486   -7.91105250     Au
    2.38393191    0.31790563    5.01943820     O
    5.15114633    2.19358483    6.14066071     H
    2.10306547    3.43668835    5.92353229     H
    4.83613739    0.43596956    6.37449051     H
    5.28449165    1.18629981    5.68578962     C
    6.37260850    0.98665728    5.58631472     H
    4.05780811    3.96223114    4.51532513     H
    1.56604344    3.17136671    4.98564203     C
    5.89211867    4.80096599    3.33013877     H
    7.58707217    4.37810152    3.24166020     H
    6.61486370    4.08048309    3.34250058     N
    1.14045425    4.10595663    4.55626904     H
    0.72780632    2.48291764    5.22990335     H
    3.78542039    3.33750962    3.63302305     C
    6.36011494    2.72699771    3.35404628     C
    4.58800120    1.08126199    4.29945970     C
    2.50642553    2.51237786    3.95099728     C
    3.10074293    1.24783802    4.52395990     N
    7.27832781    1.88478822    3.33779880     O
    4.88413508    2.28262647    3.33674097     C
    3.62558216    4.01707470    2.76439651     H
    4.86006105   -0.29772537    3.65153654     C
    4.61609374   -1.11019299    4.37237963     H
    5.93187775   -0.35400818    3.36061274     H
    1.71649666    2.10705418    2.67964691     C
    4.74291490    1.91819789    2.28610399     H
    1.25059603    3.00175348    2.20566923     H
    0.90539045    1.39231990    2.93204532     H
    4.24459573   -0.43769652    2.73370487     H
    2.38343120    1.64057071    1.92161597     H

outcell: Unit cell vectors (Ang):
        8.778588   -0.003734    0.107918
        4.385700    7.568039   -0.036078
        0.348296   -0.346904   25.844611
```

Nit8 on flat Cu(111) via NO fcc site

```
   -0.06756843   -0.03683840   -0.07454910     Cu
    2.56103933   -0.01193253   -0.00932837     Cu
    5.18951857    0.01024369    0.03769197     Cu
    7.82075463    0.03814189    0.07329210     Cu
    1.27563821    2.22423035    0.00732728     Cu
    3.89845286    2.24552876    0.04302570     Cu
    6.52970518    2.26919262    0.08511831     Cu
    9.15054073    2.29753786    0.13561664     Cu
    2.60796915    4.47327711    0.08968156     Cu
    5.23247150    4.49754598    0.10893140     Cu
    7.85572247    4.52125661    0.17577590     Cu
   10.49283612    4.54966867    0.22412325     Cu
```

3.93319113	6.72433664	0.10608213	Cu
6.57171285	6.74917202	0.14790028	Cu
9.19698155	6.77374985	0.22218304	Cu
11.83015947	6.80105100	0.26427010	Cu
1.25196424	0.71740323	-2.15445520	Cu
3.88305381	0.73224556	-2.10614219	Cu
6.50956812	0.76437217	-2.06228714	Cu
9.14040493	0.79787608	-2.02750124	Cu
2.60314591	2.96874840	-2.11127869	Cu
5.21343400	2.99665006	-2.08421101	Cu
7.83437851	3.02497082	-2.02401696	Cu
10.47884134	3.03918344	-1.95234565	Cu
3.93506703	5.20899111	-2.06661936	Cu
6.54221416	5.23887365	-2.02233665	Cu
9.18292621	5.26492012	-1.92861428	Cu
11.81421637	5.28980223	-1.88912730	Cu
5.26249528	7.46221324	-2.02219389	Cu
7.89056831	7.50600139	-1.93992697	Cu
10.52171215	7.52359538	-1.89527436	Cu
13.15126341	7.55627466	-1.85420774	Cu
-0.00416575	1.46102966	-4.32046232	Cu
2.61718012	1.45786500	-4.26925612	Cu
5.25119180	1.47402953	-4.20645819	Cu
7.88661924	1.52338859	-4.18273483	Cu
1.31500882	3.70641414	-4.22724079	Cu
3.88587606	3.69583292	-4.26018015	Cu
6.60740210	3.72223248	-4.18904906	Cu
9.22847663	3.78039149	-4.08417095	Cu
2.62564829	5.99712949	-4.14666009	Cu
5.27264455	6.05786246	-4.20003745	Cu
7.94586482	6.03126362	-4.04744329	Cu
10.55426908	6.03541831	-4.04723520	Cu
3.98465018	8.25262441	-4.14903682	Cu
6.64047883	8.26330061	-4.10132478	Cu
9.26583369	8.26307521	-4.06601685	Cu
11.89132918	8.30464010	-4.02351796	Cu
4.84484254	2.32991217	-8.22333353	H
6.36621840	3.56854917	-9.44316453	H
3.07653850	2.55048788	-8.48947971	H
3.94506976	2.88567884	-7.87855114	C
7.27312303	3.05160664	-7.23740824	H
3.74757317	2.58318192	-6.82322606	H
4.13526385	4.26459062	-10.19805983	H
8.51727052	4.11651778	-8.01576087	H
8.27654407	5.31960490	-10.34017776	O
6.15409218	4.65973519	-9.33700646	C
7.64476194	4.09751573	-7.32558781	C
7.03885224	5.30354910	-10.43112651	C
5.38336192	5.74461495	-11.68051590	H
4.62344145	4.86198245	-9.39522527	C
6.96479307	6.19546611	-12.29304826	H
6.38669024	5.83846395	-11.52957562	N
4.11762286	4.42867643	-7.98589507	C
6.56451941	5.06340023	-7.86529396	C
7.99860192	4.41741666	-6.31426425	H
5.23274816	4.97641535	-7.14982138	N

```
    5.24985334    4.62693826   -5.78867343     O
    1.98345228    4.86930973   -8.33557376     H
    4.37106902    5.93495862   -9.55933101     H
    2.79220556    5.14374798   -7.62055436     C
    2.44448117    4.85602721   -6.59890075     H
    8.04602583    6.66973552   -8.23089412     H
    7.05968042    6.53250446   -7.73806270     C
    2.92493239    6.24874306   -7.63550322     H
    6.33008443    7.24620734   -8.18254107     H
    7.16680106    6.79577273   -6.65842030     H

outcell: Unit cell vectors (Ang):
       10.517794    0.100682    0.169421
        5.346392    9.022323    0.211083
        0.380558    0.325490   26.239970
```

Nit8 on flat Cu(111) via NO hcp site

```
    0.03739750    0.02110649   -0.04893687     Cu
    2.67809625    0.04959618   -0.05965941     Cu
    5.30185182    0.08059350   -0.05857408     Cu
    7.93340210    0.10590715   -0.07713637     Cu
    1.37787448    2.28926462   -0.01818446     Cu
    4.00990806    2.31535736   -0.03709766     Cu
    6.64097512    2.33804501   -0.05947452     Cu
    9.26959884    2.36942534   -0.07099453     Cu
    2.73102292    4.54405483   -0.01128742     Cu
    5.35022961    4.56742890   -0.02913447     Cu
    7.98106781    4.59345013   -0.04377980     Cu
   10.60543128    4.62630439   -0.05252730     Cu
    4.06403842    6.79154659   -0.02394018     Cu
    6.69011662    6.82011292   -0.06161858     Cu
    9.31977313    6.84534892   -0.04386141     Cu
   11.95203115    6.87709267   -0.06715086     Cu
    1.30488445    0.74059305   -2.16554181     Cu
    3.93094886    0.78020686   -2.18284770     Cu
    6.56523084    0.78508574   -2.20012103     Cu
    9.19226917    0.82401880   -2.21568470     Cu
    2.64297115    2.99823211   -2.15247719     Cu
    5.28943549    3.01741079   -2.19327976     Cu
    7.89682179    3.04713399   -2.20392200     Cu
   10.53786036    3.07698799   -2.19560782     Cu
    4.02369691    5.25140720   -2.18067078     Cu
    6.62468055    5.26572858   -2.22016268     Cu
    9.23174949    5.31148557   -2.20134367     Cu
   11.88214817    5.33024642   -2.19616449     Cu
    5.33092094    7.49591846   -2.19620223     Cu
    7.95807539    7.52676034   -2.20295392     Cu
   10.58453132    7.56786048   -2.19585796     Cu
   13.21665883    7.58856422   -2.21486823     Cu
   -0.01725401    1.45893751   -4.30913994     Cu
    2.61535399    1.49610853   -4.32221201     Cu
    5.24243755    1.50653577   -4.33907751     Cu
    7.88510156    1.52487174   -4.35696250     Cu
    1.32673212    3.71503554   -4.28466501     Cu
```

```
    3.94438722    3.73074760   -4.27564638     Cu
    6.60638633    3.70554658   -4.37285161     Cu
    9.23551325    3.78060597   -4.28643612     Cu
    2.66106924    5.96945282   -4.27644064     Cu
    5.28076065    6.02363930   -4.37911831     Cu
    7.96294879    6.09016237   -4.36255088     Cu
   10.56933377    6.06378312   -4.30242340     Cu
    3.99714743    8.23327311   -4.31192036     Cu
    6.63075669    8.30217656   -4.31261837     Cu
    9.27343522    8.31115381   -4.32966053     Cu
   11.89506809    8.30902659   -4.35961240     Cu
    6.28296498    3.07592820   -8.39185760     H
    7.80353459    4.29925152   -9.61610172     H
    4.51258255    3.31091206   -8.63218601     H
    5.39361697    3.64267818   -8.03771582     C
    8.72514878    3.79862464   -7.44081751     H
    5.21247147    3.35300945   -6.97685577     H
    5.57691061    5.00599361  -10.37104133     H
    9.97625359    4.87136570   -8.19962469     H
    9.73732131    6.02038010  -10.51723863     O
    7.60217016    5.39349654   -9.52086419     C
    9.09941430    4.84467835   -7.51523959     C
    8.50013576    6.01269593  -10.61883491     C
    6.86619955    6.44038523  -11.90303473     H
    6.07218927    5.60681337   -9.57521871     C
    8.46489669    6.85359084  -12.49900745     H
    7.86692751    6.53411895  -11.73402281     N
    5.57183591    5.18409954   -8.15967837     C
    8.02044039    5.81020801   -8.05642568     C
    9.44745876    5.15242625   -6.49823829     H
    6.69317394    5.73189654   -7.33077437     N
    6.71329087    5.38110577   -5.97684000     O
    3.43272280    5.62168720   -8.48421452     H
    5.82443051    6.67977878   -9.74572608     H
    4.25120157    5.89969367   -7.78241382     C
    3.92259819    5.61313100   -6.75471347     H
    9.49053688    7.42271326   -8.45170714     H
    8.50835753    7.28343235   -7.95158685     C
    4.38209818    7.00480225   -7.79745159     H
    7.76969270    7.98437150   -8.40136903     H
    8.61702223    7.56103223   -6.87574561     H

outcell: Unit cell vectors (Ang):
       10.520354    0.114696   -0.057562
        5.357351    9.027859   -0.008621
       -0.159495    0.031768   25.926922
```

Nit8 on flat Cu(111) via >CO

```
    0.05827722    0.03461538   -0.05990058     Cu
    2.69808060    0.08393029   -0.03658407     Cu
    5.32760569    0.12860308   -0.04597111     Cu
    7.95543925    0.16978584   -0.07608669     Cu
    1.41787974    2.30075748   -0.03991519     Cu
    4.05011461    2.34862982   -0.03673485     Cu
```

6.68156851	2.39212181	-0.05885631	Cu
9.31046097	2.43174742	-0.08585320	Cu
2.77436381	4.56594739	-0.05584779	Cu
5.40253029	4.61123213	-0.05272527	Cu
8.03673410	4.65544598	-0.06067496	Cu
10.67018217	4.70209311	-0.07788267	Cu
4.12466610	6.82890336	-0.08508762	Cu
6.75875051	6.87547518	-0.06975122	Cu
9.39093099	6.92107269	-0.06665052	Cu
12.02169037	6.96423644	-0.09560266	Cu
1.37489022	0.80036328	-2.18386642	Cu
4.00511585	0.84634830	-2.18321538	Cu
6.63615342	0.88545859	-2.20338632	Cu
9.27148020	0.92508545	-2.22334175	Cu
2.72605565	3.05757818	-2.18228903	Cu
5.35892563	3.10750190	-2.19136159	Cu
7.99016619	3.15096736	-2.20419541	Cu
10.63124666	3.18972995	-2.21531216	Cu
4.08666139	5.32360672	-2.20964752	Cu
6.71668194	5.36791475	-2.20577888	Cu
9.35175378	5.41125552	-2.19872595	Cu
11.98310009	5.45680396	-2.22992494	Cu
5.44100928	7.57706038	-2.22859966	Cu
8.06982135	7.64122746	-2.20150635	Cu
10.70232109	7.68100078	-2.22837526	Cu
13.33180088	7.72152304	-2.25567137	Cu
0.00421284	1.47851204	-4.34326013	Cu
2.63318213	1.52821496	-4.33436602	Cu
5.26525291	1.56995852	-4.33341401	Cu
7.90603275	1.60332258	-4.35346178	Cu
1.35971966	3.74339006	-4.34716785	Cu
3.97859909	3.78465605	-4.31717085	Cu
6.63370729	3.80931696	-4.31825978	Cu
9.26237468	3.86844528	-4.32396867	Cu
2.71627191	6.00065314	-4.37013908	Cu
5.34002815	6.05100669	-4.35536217	Cu
8.03793266	6.13404277	-4.29616206	Cu
10.62368396	6.13913436	-4.35793840	Cu
4.06716014	8.26727315	-4.38155080	Cu
6.69777214	8.32287936	-4.34641712	Cu
9.33461714	8.37399377	-4.36149559	Cu
11.96474382	8.40299836	-4.39640845	Cu
7.58417620	7.22772701	-12.35483870	H
8.40736951	7.35148458	-10.75601151	H
8.23763492	6.68792855	-11.63299134	C
9.22331432	6.50634817	-12.11645796	H
7.38721158	6.59457734	-8.68811077	H
5.77121801	6.34273970	-10.52623292	H
9.77270835	6.16606285	-8.45888591	H
7.61642944	5.32105897	-11.22185000	C
6.39555687	5.45802534	-10.26925127	C
7.00598590	5.55522414	-8.84407650	C
6.60873902	4.97263892	-13.15216518	H
4.28575391	5.45735735	-8.73204302	H
6.07597953	5.34620343	-7.63721373	C
9.46457548	5.17105402	-8.06553967	C

```
     4.72464600    5.32684142   -7.82066104     N
     7.33567865    4.46371976  -12.47996777     C
     9.20334762    5.28617530   -6.98949255     H
     6.57798962    5.24740454   -6.48466941     O
     8.58767228    4.59319089  -10.33210975     N
     4.13249357    5.27016463   -6.97760553     H
     8.28248664    4.30105640  -13.04000544     H
     8.25996477    4.60240880   -8.85633752     C
     5.75888793    4.54726096  -10.36199330     H
     9.71008375    4.14663013  -10.77571670     O
    10.33540696    4.48505831   -8.15378514     H
     6.92567747    3.46552267  -12.20633421     H
     7.95965624    3.14073638   -8.41796128     C
     7.81525347    3.06964860   -7.31674301     H
     7.05370475    2.73357066   -8.92246842     H
     8.82360372    2.50069040   -8.70373580     H

outcell: Unit cell vectors (Ang):
       10.527072    0.178950   -0.031739
        5.418008    9.056976   -0.042882
       -0.086545   -0.071476   26.547710
```

Nit8 on Cu adatom on-top via NO

```
     5.35346861    3.05563748    2.08362507     Cu
     0.05965271    0.02060673    0.13529507     Cu
     2.68410170    0.05785291    0.13215215     Cu
     5.30998593    0.09203731    0.14253471     Cu
     7.93817126    0.11905379    0.11148044     Cu
     1.40171454    2.27988098    0.11427678     Cu
     4.01842602    2.30763632    0.12630258     Cu
     6.66435674    2.33701311    0.08595671     Cu
     9.28049512    2.37841989    0.09458399     Cu
     2.74690098    4.53348936    0.12278253     Cu
     5.36989845    4.57673074    0.10954373     Cu
     7.99746668    4.60300108    0.10896476     Cu
    10.62221832    4.63947502    0.09706921     Cu
     4.09072746    6.79010495    0.08969636     Cu
     6.71453411    6.82637650    0.09263191     Cu
     9.33942196    6.86404549    0.09195084     Cu
    11.96772266    6.89521383    0.08471400     Cu
     1.37420053    0.74887766   -2.01860331     Cu
     4.00073579    0.78480668   -2.02391469     Cu
     6.62448950    0.81554948   -2.03771432     Cu
     9.25301418    0.85104069   -2.03582937     Cu
     2.71827524    3.00523607   -2.03782694     Cu
     5.33874795    3.04008801   -2.06708981     Cu
     7.96657738    3.07502661   -2.05080151     Cu
    10.59457222    3.11117793   -2.04842745     Cu
     4.06172209    5.26032428   -2.05163878     Cu
     6.68388837    5.29390579   -2.05001210     Cu
     9.31148016    5.33194842   -2.04771464     Cu
    11.94113676    5.36378751   -2.05278435     Cu
     5.40648590    7.51790361   -2.05912092     Cu
     8.03105275    7.55361488   -2.06001825     Cu
```

```
   10.65672136    7.58982498   -2.06161841     Cu
   13.28277657    7.61909677   -2.07353813     Cu
    0.02792904    1.45277003   -4.17055009     Cu
    2.65132612    1.48509640   -4.17976616     Cu
    5.27787616    1.51789587   -4.18528088     Cu
    7.90738243    1.55328458   -4.19206088     Cu
    1.36946088    3.70989910   -4.18960750     Cu
    3.99435278    3.74334941   -4.19517322     Cu
    6.62500830    3.77906852   -4.20184911     Cu
    9.25069512    3.81351675   -4.19609586     Cu
    2.71456819    5.96649600   -4.20098408     Cu
    5.34083521    6.00243225   -4.20457035     Cu
    7.96836589    6.03689186   -4.20009588     Cu
   10.59139070    6.06787245   -4.20618318     Cu
    4.05728640    8.22082966   -4.21338809     Cu
    6.68504474    8.25714534   -4.20934632     Cu
    9.30909081    8.28791944   -4.21759921     Cu
   11.93663020    8.32242420   -4.22525423     Cu
    6.06201522    2.98062705    3.90231335     O
    6.85181900    5.43717288    6.88438373     H
    7.08165822    3.65049965    6.96189499     H
    6.75742896    4.49029718    6.30721366     C
    7.44963497    4.53449648    5.43836937     H
    5.35706979    2.13972420    7.61676151     H
    4.54986733    4.44256339    7.87764309     H
    6.64188201    0.98132577    5.93753788     H
    5.29891062    4.30897727    5.79437300     C
    4.30465751    3.91816407    6.92671687     C
    4.42462489    2.37519647    7.04799886     C
    4.87629641    6.46847043    5.62234924     H
    2.49920009    3.36263827    8.66573490     H
    3.33025929    1.59953273    7.82034082     C
    5.65719554    0.68839185    5.50840444     C
    2.46532054    2.34631604    8.60005013     N
    4.86048084    5.55561291    4.98581976     C
    5.25155868   -0.16540369    6.09460233     H
    3.26164142    0.36117296    7.77463476     O
    5.19901432    3.09942996    4.91714578     N
    1.76463303    1.84125523    9.14617299     H
    5.54857423    5.71833979    4.12613425     H
    4.64431468    1.85856765    5.57493939     C
    3.27239872    4.21346913    6.62810573     H
    5.82780166    0.37093410    4.45655100     H
    3.83302166    5.42289523    4.57987533     H
    3.32581866    1.47699272    4.84307231     C
    2.90878798    0.53187056    5.25179976     H
    2.55844626    2.27698544    4.94586417     H
    3.52687466    1.33973127    3.75502042     H

outcell: Unit cell vectors (Ang):
       10.502702    0.137504   -0.013707
        5.374083    9.026978   -0.053907
       -0.044335   -0.139743   26.971244
```

Nit8 on Cu adatom on-top via >CO

5.62629493	3.32582693	2.04318777	Cu
0.00273460	0.06070168	0.04266289	Cu
2.62603627	0.09321784	0.08050635	Cu
5.24322605	0.11585127	0.11385830	Cu
7.86251066	0.13951244	0.11843997	Cu
1.34254444	2.31633636	0.07471079	Cu
3.97105386	2.35504959	0.18696038	Cu
6.60057858	2.34609334	0.04111070	Cu
9.19158879	2.40046441	0.16072973	Cu
2.66890794	4.57717286	0.09221719	Cu
5.27801180	4.62964935	0.03176450	Cu
7.85443610	4.59917103	0.24520364	Cu
10.51097582	4.65602865	0.19891043	Cu
3.99944782	6.83147743	0.07539958	Cu
6.62193633	6.85671428	0.11775896	Cu
9.22999164	6.87840730	0.16229561	Cu
11.85557653	6.91492686	0.18992953	Cu
1.33619451	0.79422851	-2.08240136	Cu
3.95789394	0.82873846	-2.03295752	Cu
6.57629470	0.84559966	-2.06721462	Cu
9.19089434	0.88026642	-2.01209165	Cu
2.67893050	3.04442236	-2.03510404	Cu
5.28161763	3.07167296	-2.08786378	Cu
7.91234173	3.10657955	-2.04139739	Cu
10.52727359	3.13245140	-1.94624965	Cu
3.99901312	5.30489886	-2.09251205	Cu
6.62966990	5.32956892	-2.05597315	Cu
9.23110760	5.35174306	-1.94991211	Cu
11.85600082	5.38549110	-1.93149584	Cu
5.33631553	7.55493274	-2.06194063	Cu
7.95454961	7.58815411	-2.01719325	Cu
10.56899879	7.61485232	-1.98569941	Cu
13.18660980	7.64090012	-1.96988411	Cu
0.02589508	1.50138084	-4.25351260	Cu
2.64108097	1.52336402	-4.21556251	Cu
5.25656043	1.54150525	-4.20497485	Cu
7.88268567	1.57414575	-4.21275179	Cu
1.35532081	3.74705254	-4.21368280	Cu
3.96875238	3.77223862	-4.21511689	Cu
6.59696862	3.80562370	-4.19478343	Cu
9.21675797	3.84029856	-4.13754415	Cu
2.68394410	6.00135336	-4.23329732	Cu
5.30761038	6.03759971	-4.21402751	Cu
7.93132029	6.06805676	-4.16217376	Cu
10.54203942	6.08254011	-4.11633303	Cu
4.02062921	8.25846891	-4.22688384	Cu
6.64209513	8.29459896	-4.18316449	Cu
9.25703155	8.31484204	-4.14760001	Cu
11.87735189	8.33618991	-4.14117214	Cu
5.29990295	2.86131927	4.00411244	O
6.37081094	5.08294775	4.55534100	H
5.96898647	4.59130281	5.35944730	N
3.58158634	2.83946254	6.12705562	H
5.35402730	3.39149293	5.14730526	C

```
    4.01938025    0.55178407    4.48640073     H
    5.95506872    5.05682065    6.26745689     H
    2.86225494    0.56303261    5.87473894     H
    4.66944622    2.69136303    6.33492474     C
    2.34654692    2.37761312    8.13908927     H
    3.90495715    0.32299026    5.56799231     C
    4.47452122    4.18372543    7.98474386     H
    4.97491222    3.21269380    7.76866302     C
    2.95798895    2.18818370    9.05000202     C
    4.92260830    1.13961027    6.39759913     C
    2.75571560    3.00409764    9.77939403     H
    4.07008944   -0.76221112    5.74732285     H
    6.56252218    0.79699829    4.95983508     H
    2.62459798    1.22216267    9.49063097     H
    4.47477982    2.08582865    8.72057607     C
    6.07189862    3.35033575    7.91003151     H
    6.37698794    0.71917334    6.05237996     C
    4.69628957    0.87119330    7.86480736     N
    7.12578011    1.34581964    6.58756424     H
    4.50095804   -0.31967393    8.31493981     O
    6.52440779   -0.33544051    6.37521142     H
    5.29999810    1.93624379   10.02122450     C
    5.10167005    2.77787012   10.72117688     H
    6.39084792    1.90471097    9.80458416     H
    5.02492597    0.97999405   10.52040780     H

outcell: Unit cell vectors (Ang):
       10.472812    0.114139    0.132861
        5.330370    9.019855    0.057923
        0.324987   -0.029168   27.517733
```

Nit8 on Cu adatom on-top via -NH_2

```
    5.24353818    2.96246619    1.90791694     Cu
    0.03783340    0.03821133    0.04880465     Cu
    2.65753906    0.07188527    0.02821818     Cu
    5.27534247    0.11917334    0.02793198     Cu
    7.90542857    0.13964050   -0.01466672     Cu
    1.36731623    2.29134641   -0.00381466     Cu
    3.95947341    2.31594030   -0.07808111     Cu
    6.63159044    2.35331013   -0.05616004     Cu
    9.24286421    2.39255014   -0.05499842     Cu
    2.72071691    4.53796811   -0.00211559     Cu
    5.34478025    4.57618527   -0.02629993     Cu
    7.96725128    4.60512348   -0.03483755     Cu
   10.58846438    4.63888603   -0.06036491     Cu
    4.06515816    6.79190799   -0.04340343     Cu
    6.68505279    6.82739922   -0.05329022     Cu
    9.30926923    6.86156946   -0.06687768     Cu
   11.93068178    6.89857064   -0.09243938     Cu
    1.29298938    0.75290966   -2.12848294     Cu
    3.91358499    0.78368961   -2.17432688     Cu
    6.53449050    0.82174110   -2.18814648     Cu
    9.15849149    0.85970470   -2.19067343     Cu
    2.62923021    3.01065301   -2.19183715     Cu
```

5.25524323	3.04365322	-2.22786899	Cu
7.87630247	3.07840555	-2.22104151	Cu
10.49867953	3.11371110	-2.22891743	Cu
3.97707710	5.25851557	-2.18130333	Cu
6.59623758	5.29468780	-2.18982946	Cu
9.21794492	5.32954155	-2.19766894	Cu
11.84251751	5.36405193	-2.22312259	Cu
5.31818806	7.51387401	-2.20015676	Cu
7.93949982	7.54737193	-2.21431850	Cu
10.56020771	7.58559364	-2.22709407	Cu
13.18231804	7.61708130	-2.25876649	Cu
-0.06007858	1.46623924	-4.28270985	Cu
2.55688313	1.49666893	-4.31178013	Cu
5.18152047	1.53149251	-4.33271618	Cu
7.80667986	1.56689561	-4.34738764	Cu
1.27674813	3.72336695	-4.31701220	Cu
3.89977854	3.75883258	-4.33968972	Cu
6.52698867	3.79535655	-4.35835392	Cu
9.14931999	3.82748733	-4.36828276	Cu
2.62196834	5.97623551	-4.33544169	Cu
5.24436491	6.01205561	-4.35710390	Cu
7.86775054	6.04371209	-4.36369678	Cu
10.48662113	6.07677551	-4.38269704	Cu
3.96316794	8.22226646	-4.37006541	Cu
6.58630618	8.25721318	-4.37973108	Cu
9.20714396	8.28615630	-4.40671433	Cu
11.83025550	8.32197624	-4.42636606	Cu
5.11626223	1.25828374	5.23070357	O
6.00745075	3.29557913	4.34036353	H
5.03367380	3.21417367	4.00033199	N
2.67501201	1.02112747	4.30542375	H
4.40173322	2.11586445	4.71624473	C
3.40313282	0.25648534	6.99825960	H
4.53876326	4.11674032	4.07551970	H
1.82445705	-0.15145164	6.22174583	H
2.86617077	2.02766958	4.75104910	C
0.39012424	0.77330510	3.76423865	H
2.35032059	0.58796645	6.86559193	C
2.01133409	2.93392458	2.90089137	H
1.97800843	3.06535806	4.00759398	C
-0.22966947	1.68958007	3.89252917	C
2.31137496	1.99528380	6.22802830	C
-0.57746527	2.00089604	2.87995433	H
1.83189452	0.61679818	7.84887466	H
3.97828447	2.72850822	7.49135170	H
-1.11371400	1.42220991	4.51524589	H
0.54949244	2.83862608	4.59513496	C
2.29213159	4.11356048	4.22743958	H
2.95479053	3.03763413	7.18509988	C
0.88219781	2.40355549	5.99706933	N
3.00247299	4.05349774	6.73089320	H
-0.00342175	2.30752964	6.92562336	O
2.31813745	3.11309595	8.09483067	H
-0.33288196	4.10971136	4.66184066	C
-0.66077462	4.41550397	3.64255654	H
0.20189074	4.96332273	5.13597286	H

-1.22996018	3.89346100	5.28701265	H

outcell: Unit cell vectors (Ang):

10.486986	0.137366	-0.071873
5.366889	9.012429	-0.123849
-0.197653	-0.274203	27.638569

Nit8 on Cu step on-top via NO

8.02331230	0.10225090	-0.20760084	Cu
6.66214159	2.35181506	-0.00431723	Cu
9.28335957	2.35897297	-0.23709650	Cu
5.38399831	4.61627698	-0.15251800	Cu
7.96555042	4.61703133	-0.12757386	Cu
10.52815622	4.60381700	-0.28184435	Cu
4.08569863	6.81632120	-0.12942552	Cu
6.66227351	6.84568322	-0.20274843	Cu
9.23761318	6.82489998	-0.29187986	Cu
11.83357405	6.81356161	-0.33943167	Cu
1.44566554	0.81344497	-1.85372421	Cu
4.03030771	0.81114581	-1.92497860	Cu
6.58018842	0.82636022	-2.16664053	Cu
9.20555629	0.82557310	-2.31681065	Cu
2.74439061	3.05531393	-1.91561306	Cu
5.28685966	3.02593579	-2.12617634	Cu
7.87652759	3.04927691	-2.26135723	Cu
10.51910597	3.03961136	-2.33638717	Cu
4.00971179	5.27589021	-2.20541501	Cu
6.60426777	5.29846277	-2.30328444	Cu
9.18019726	5.28799691	-2.38344689	Cu
11.77789253	5.27804062	-2.41061256	Cu
5.31895699	7.54784593	-2.27300945	Cu
7.89441952	7.57616063	-2.32937077	Cu
10.46893926	7.54856225	-2.40464906	Cu
13.04748774	7.52837037	-2.47227044	Cu
0.14413850	1.53614457	-4.24899135	Cu
2.70245046	1.53708462	-4.06692487	Cu
5.26586310	1.53701766	-4.28843419	Cu
7.84936084	1.54512294	-4.44723637	Cu
1.43512660	3.76306630	-4.29578929	Cu
3.98369103	3.76132238	-4.29216187	Cu
6.56221503	3.77037141	-4.40905175	Cu
9.14747062	3.77188913	-4.49885496	Cu
2.71039082	6.00864279	-4.40365626	Cu
5.27454334	6.00913834	-4.44510805	Cu
7.85604720	6.01379227	-4.50945324	Cu
10.43646188	6.01018606	-4.58114905	Cu
3.99005482	8.24316187	-4.44424878	Cu
6.56743772	8.25419465	-4.44959075	Cu
9.14104733	8.25791646	-4.51331160	Cu
11.72353534	8.25206514	-4.59437264	Cu
3.81679896	3.70565378	6.25042742	O
3.81752329	1.99026441	8.08709533	H
4.19441021	1.65303504	7.19924350	N
3.77006546	1.86262972	4.18083074	H

```
    4.21308543    2.53553217    6.13393208     C
    4.20312243    4.63727117    3.78292624     H
    4.48651921    0.67904503    7.12873505     H
    4.14576805    3.45183498    2.41640541     H
    4.70768046    1.98294466    4.77535776     C
    4.18574727    0.47707648    2.28462527     H
    4.81936590    3.98790306    3.12358360     C
    4.80617433   -0.24428281    4.90114094     H
    5.47467574    0.63269445    4.74879958     C
    5.20103507    0.02401923    2.24726866     C
    5.62447942    2.99102316    3.98863719     C
    5.09718476   -1.08325648    2.33300711     H
    5.51039576    4.62166947    2.51917755     H
    6.12808534    4.53264213    5.48655678     H
    5.62612599    0.23611472    1.23650215     H
    6.14955564    0.58408929    3.34602890     C
    6.26003089    0.60794935    5.53905697     H
    6.64348738    3.75218371    4.88659484     C
    6.38570502    2.04087229    3.10917998     N
    7.17064020    3.06397882    5.58503926     H
    7.08106618    2.48107208    2.07745647     O
    7.40783129    4.23199549    4.23622624     H
    7.50528455   -0.16358197    3.33032142     C
    7.35970944   -1.25974671    3.45694388     H
    8.17911113    0.20733639    4.13522842     H
    8.01370519   -0.00222014    2.34834817     H

outcell: Unit cell vectors (Ang):
       10.302534    0.005819   -0.226445
        5.156228    8.928201   -0.154080
       -0.585593   -0.118382   29.295077
```

Nit8 on Cu step on-top via >CO

```
    8.03691594    0.14244341   -0.14617052     Cu
    6.69984981    2.39179942   -0.07272644     Cu
    9.29004299    2.40517617   -0.15003442     Cu
    5.43373085    4.67408558   -0.20215468     Cu
    8.00490151    4.64738006   -0.07691516     Cu
   10.56677174    4.63742848   -0.19789095     Cu
    4.12031883    6.85942367   -0.18240169     Cu
    6.71287574    6.87864991   -0.20196546     Cu
    9.28749579    6.86443091   -0.23483448     Cu
   11.86770867    6.86514210   -0.24586656     Cu
    1.52997449    0.88807686   -1.96436287     Cu
    4.10919554    0.88607060   -2.00391180     Cu
    6.66764411    0.87949417   -2.20408458     Cu
    9.28518261    0.88857848   -2.23495938     Cu
    2.82191455    3.12661404   -2.01673041     Cu
    5.36326969    3.09254307   -2.20483768     Cu
    7.95450727    3.11309461   -2.23340620     Cu
   10.59466035    3.10423432   -2.24836906     Cu
    4.08823496    5.34241901   -2.26935772     Cu
    6.69095241    5.36234685   -2.31732360     Cu
    9.26867842    5.35874049   -2.33429253     Cu
```

```
   11.85456743    5.34543374   -2.31605763     Cu
    5.40226515    7.61113106   -2.28995591     Cu
    7.98263519    7.63184977   -2.29594940     Cu
   10.55610257    7.60995663   -2.33592389     Cu
   13.13217598    7.58883553   -2.37760482     Cu
    0.24015387    1.59358435   -4.31770164     Cu
    2.80696545    1.59794853   -4.16264504     Cu
    5.37321834    1.58884249   -4.34754666     Cu
    7.96043391    1.59494690   -4.41499217     Cu
    1.52671493    3.82526364   -4.36611557     Cu
    4.08489060    3.82346685   -4.36743295     Cu
    6.66666835    3.82634852   -4.42740772     Cu
    9.25147924    3.82544356   -4.42348845     Cu
    2.80899249    6.06522196   -4.47078029     Cu
    5.38034844    6.06849728   -4.47836961     Cu
    7.96366991    6.07261186   -4.48852148     Cu
   10.54412439    6.06602391   -4.52603875     Cu
    4.09766269    8.29933762   -4.49495120     Cu
    6.67478462    8.31080764   -4.44321688     Cu
    9.25294340    8.31024085   -4.47046289     Cu
   11.82980589    8.29980733   -4.54206554     Cu
    5.82630484    1.85972784    1.77074238     O
    7.88410061    3.13030047    2.49663874     H
    7.30901316    2.76817093    3.27512029     N
    4.35710748    2.33127359    3.99834675     H
    6.16716899    2.09482426    2.96365725     C
    3.62692709    0.45739740    1.95688467     H
    7.54736629    3.02066409    4.23497476     H
    2.60350536    0.79932281    3.40663179     H
    5.22374455    1.63198534    4.08588759     C
    3.03389730    2.18688834    5.99433290     H
    3.39258102    0.13115051    2.99314810     C
    5.78733077    2.69907589    5.96442562     H
    5.73450537    1.66577721    5.55319872     C
    3.45898733    1.55897032    6.80874192     C
    4.66776939    0.17521991    3.86852551     C
    3.68432208    2.21993789    7.67512385     H
    2.98696296   -0.90457864    2.97400044     H
    5.94295654   -0.68138222    2.27170815     H
    2.68137044    0.82295715    7.11244693     H
    4.72382867    0.78317213    6.34244419     C
    6.75184522    1.21638408    5.62665691     H
    5.72555311   -0.83897884    3.35224749     C
    4.31327343   -0.20277932    5.28416571     N
    6.68366168   -0.76919429    3.91598082     H
    3.55749207   -1.21064766    5.55260932     O
    5.32411796   -1.86843193    3.48166606     H
    5.34616557    0.00878935    7.52738946     C
    5.58906909    0.69352597    8.36958732     H
    6.27561760   -0.51881702    7.21780004     H
    4.62044144   -0.75722991    7.88120725     H

outcell: Unit cell vectors (Ang):
       10.309495    0.001160   -0.062917
        5.155640    8.932998   -0.127625
       -0.179397   -0.307433   29.670217
```

Nit8 on Cu step on-top via -NH_2

8.00372352	0.16783726	-0.23122191	Cu
6.74963231	2.38485458	-0.31307465	Cu
9.30264891	2.40545761	-0.28498649	Cu
5.42510279	4.61455443	-0.24810689	Cu
8.03066932	4.64145865	-0.29426824	Cu
10.58514749	4.64206417	-0.32492179	Cu
4.13934783	6.90513615	-0.29493989	Cu
6.72309115	6.91075993	-0.30046220	Cu
9.30141550	6.86450486	-0.34613664	Cu
11.88231800	6.86742202	-0.36076430	Cu
1.55151358	0.89773901	-2.00693410	Cu
4.13640550	0.90014967	-2.05777242	Cu
6.68371291	0.87239425	-2.33926473	Cu
9.30606792	0.88726036	-2.34396989	Cu
2.84476117	3.13523509	-2.08651501	Cu
5.38015915	3.10921687	-2.32605323	Cu
7.99996942	3.12420781	-2.43102533	Cu
10.61791573	3.10655265	-2.37796370	Cu
4.11130704	5.34510907	-2.34359100	Cu
6.69234978	5.36222921	-2.39696808	Cu
9.29059673	5.36254425	-2.48156052	Cu
11.87744750	5.34532595	-2.44395644	Cu
5.42270348	7.60584666	-2.40241457	Cu
7.99919000	7.62822533	-2.41067089	Cu
10.56974042	7.59808459	-2.46220289	Cu
13.14336202	7.58008128	-2.52906132	Cu
0.26046944	1.59432163	-4.39927531	Cu
2.81929931	1.59636429	-4.23083529	Cu
5.37841157	1.58811454	-4.45494963	Cu
7.97479889	1.58883258	-4.53603222	Cu
1.54664114	3.82090365	-4.45414376	Cu
4.09224529	3.81773746	-4.47719197	Cu
6.67669988	3.82427645	-4.54543274	Cu
9.27089376	3.82231848	-4.58947134	Cu
2.82386220	6.05571976	-4.56098762	Cu
5.39156553	6.05557929	-4.58578209	Cu
7.96937369	6.05976275	-4.60526115	Cu
10.55514705	6.05486366	-4.66900846	Cu
4.10726747	8.28263803	-4.60211727	Cu
6.68750635	8.29709156	-4.56762133	Cu
9.26017871	8.29383615	-4.59754391	Cu
11.83809046	8.27701016	-4.70572602	Cu
6.34203888	6.42293179	2.69033679	O
4.30900620	5.10145218	2.12326476	H
5.15971201	4.52237558	2.15449948	N
8.26647205	4.54274535	2.45754424	H
6.28187655	5.18520698	2.71153009	C
8.60267109	6.78953145	4.21943011	H
5.00297010	3.53758686	2.39877868	H
9.89830898	5.56419167	3.92197242	H
7.45549875	4.31783538	3.20170001	C
9.99543639	2.84229901	2.68671515	H
9.05320396	5.84400630	4.59132798	C
7.30351918	2.32507534	2.23690658	H

```
     7.27142219    2.77865560    3.25920363     C
     9.75325982    2.00458197    3.38165034     C
     7.98176899    4.72939246    4.62587155     C
     9.69203393    1.07010562    2.77766625     H
     9.46265444    5.99334257    5.61452845     H
     6.42406586    6.08777152    5.41973376     H
    10.58991774    1.90422016    4.10917509     H
     8.42886123    2.26190820    4.15986254     C
     6.29761708    2.50602310    3.73127433     H
     6.85335548    5.08524787    5.63551513     C
     8.62657112    3.44144008    5.07332593     N
     6.02841047    4.33772718    5.61548011     H
     9.38463007    3.38740788    6.11011065     O
     7.28146021    5.08868607    6.66218257     H
     8.05342207    1.02827555    5.01329730     C
     7.97432940    0.11871469    4.37715028     H
     7.08155908    1.18297827    5.53410260     H
     8.83475171    0.86309503    5.78754256     H

outcell: Unit cell vectors (Ang):
       10.306013   -0.004926   -0.110387
        5.148963    8.911446   -0.166882
       -0.312508   -0.351835   30.317295
```

Nit8 w/o O on Cu step on-top via NH_2

```
     8.07317541    0.18187951   -0.13497305     Cu
     6.77590653    2.44074826    0.07411792     Cu
     9.36283799    2.42512981   -0.20852262     Cu
     5.48096723    4.70795705   -0.25583951     Cu
     8.05579358    4.70248357   -0.17766321     Cu
    10.60356870    4.67578338   -0.29351124     Cu
     4.15080412    6.89344502   -0.25058324     Cu
     6.74715456    6.94909866   -0.28235257     Cu
     9.31517351    6.90124626   -0.31823138     Cu
    11.88339368    6.91295977   -0.33015154     Cu
     1.53796420    0.90901072   -1.97260275     Cu
     4.09660807    0.90869496   -2.19026777     Cu
     6.66272981    0.90458326   -2.17169676     Cu
     9.28036520    0.91247818   -2.26107862     Cu
     2.82755405    3.14021203   -2.06822378     Cu
     5.37800473    3.10345885   -2.20068923     Cu
     7.95072155    3.12832308   -2.23468107     Cu
    10.60390718    3.13060658   -2.33234204     Cu
     4.09885077    5.35483890   -2.30723523     Cu
     6.69698351    5.38723021   -2.36844962     Cu
     9.27316004    5.38234294   -2.42700425     Cu
    11.85502218    5.37932994   -2.41591391     Cu
     5.41203321    7.63646057   -2.36270836     Cu
     7.99532080    7.65882046   -2.38390904     Cu
    10.55553038    7.64177601   -2.43431087     Cu
    13.13250996    7.62604232   -2.45447370     Cu
     0.22067690    1.60254932   -4.35039220     Cu
     2.77162454    1.61668862   -4.28089274     Cu
     5.35815834    1.60812294   -4.38115009     Cu
```

```
    7.93474838    1.61682027   -4.41438914     Cu
    1.50984575    3.83921907   -4.45616378     Cu
    4.06885723    3.83476661   -4.38913205     Cu
    6.65106405    3.84301741   -4.44768049     Cu
    9.22744055    3.84557743   -4.49826590     Cu
    2.80374684    6.08266488   -4.52555122     Cu
    5.36751498    6.08308917   -4.53348353     Cu
    7.94700698    6.09057428   -4.55820662     Cu
   10.51984580    6.08788319   -4.62675211     Cu
    4.08770625    8.31302751   -4.56647608     Cu
    6.65979532    8.32722773   -4.52512566     Cu
    9.23232491    8.32639008   -4.61621445     Cu
   11.81650186    8.32945849   -4.61451737     Cu
    6.45036238    0.67087477    5.76776977     H
    8.22740383    2.61793538    4.32498429     H
    6.56754874    1.18719469    3.28716980     H
    5.57594496    1.11772219    6.29057976     C
    4.91828798    0.29149623    6.64198161     H
    5.95316685    1.67410355    7.17725242     H
    8.23941050    3.45560623    2.71699328     H
    7.78511505    3.45067592    3.73431302     C
    5.75291693    1.92725750    3.07715290     C
    4.31631681    0.45702087    3.97521597     H
    5.58611716    1.83248903    1.55128648     C
    8.03733938    4.40165886    4.25423880     H
    4.51627330    1.14496993    1.15628642     N
    4.51171306    1.55277747    3.95287656     C
    4.79949170    2.10556516    5.37579418     C
    6.24654454    3.31067823    3.65293464     C
    4.34699579    0.97417926    0.14109245     H
    3.83189912    0.70605899    1.79275883     H
    5.70011459    3.26246065    5.05677383     N
    6.05430914    4.11938694    5.94814393     O
    2.89312529    1.78742980    6.43459568     H
    3.54348412    2.63105674    6.11161442     C
    3.59807065    2.04946235    3.54981132     H
    5.62625678    4.54835478    2.95891719     C
    3.85839370    3.20845686    7.00861175     H
    6.13123357    4.74209800    1.97886774     H
    5.77776405    5.44075446    3.60671119     H
    2.94864243    3.30774273    5.45900914     H
    4.53611389    4.42732153    2.77344921     H

outcell: Unit cell vectors (Ang):
       10.297401    0.014495   -0.080191
        5.160950    8.940477   -0.203453
       -0.224652   -0.526841   29.182353
```

Nit8 w/o NH_2 on Cu step on-top via CO

```
    8.11888055    0.22873278   -0.64854175     Cu
    6.87074191    2.48071031   -0.50414553     Cu
    9.47003292    2.44391326   -0.75904906     Cu
    5.59067984    4.74355422   -0.68154224     Cu
    8.16008281    4.75539069   -0.67640715     Cu
```

10.70069660	4.71265758	-0.87821633	Cu
4.25149294	6.91447215	-0.72136495	Cu
6.83627346	7.00296486	-0.79049193	Cu
9.40981943	6.98494100	-0.89131120	Cu
11.97445411	6.91209193	-0.91477170	Cu
1.58000434	0.90949996	-2.23659529	Cu
4.18022105	0.90559423	-2.35838708	Cu
6.72542995	0.92245475	-2.66193089	Cu
9.33392968	0.91078764	-2.79241751	Cu
2.88244106	3.15528421	-2.39301875	Cu
5.42332708	3.12075398	-2.64062328	Cu
8.02233389	3.14070513	-2.79777326	Cu
10.65879568	3.11946315	-2.87287345	Cu
4.15884130	5.35291510	-2.75656889	Cu
6.75372492	5.37992452	-2.85719596	Cu
9.32072046	5.37790122	-2.95853175	Cu
11.91560980	5.36064258	-3.00667384	Cu
5.46140592	7.61426689	-2.86682625	Cu
8.02984415	7.66261332	-2.94404402	Cu
10.60952240	7.61620000	-3.02694801	Cu
13.18072058	7.59687940	-3.05456738	Cu
0.27476299	1.58981366	-4.76823012	Cu
2.80763854	1.58910540	-4.48564458	Cu
5.37125439	1.58769249	-4.74708410	Cu
7.95981003	1.59765073	-4.94854873	Cu
1.55574261	3.80927217	-4.89122294	Cu
4.08733509	3.80015177	-4.82341364	Cu
6.66419682	3.81406515	-4.94944120	Cu
9.25757162	3.82237224	-5.04710874	Cu
2.83778162	6.04602863	-5.02995503	Cu
5.39190381	6.04584162	-5.00923354	Cu
7.96950047	6.05249459	-5.10177313	Cu
10.54328035	6.04620640	-5.18612759	Cu
4.12104838	8.26981551	-5.08457786	Cu
6.68249371	8.28165459	-5.05877727	Cu
9.24972875	8.28674866	-5.12446915	Cu
11.83205764	8.27927928	-5.21665578	Cu
3.53453324	-0.21885333	2.91308696	H
5.32432401	1.25409181	4.92197629	H
5.68937137	0.94362328	2.51714099	H
2.62860728	0.33309768	2.57791005	C
2.20038296	-0.21566309	1.70446651	H
1.88669334	0.32945018	3.40657889	H
6.63260338	2.49130107	4.76444801	H
5.53174507	2.33508792	4.75902698	C
5.42345082	1.97180187	2.16690260	C
7.70355757	2.78792505	2.20931599	O
4.24686060	1.04465535	0.52168829	H
6.75219386	2.46730750	1.49323736	C
5.06755265	2.90171342	5.59620863	H
4.19393641	1.89775798	1.23511505	C
2.96329781	1.79797299	2.17032282	C
4.95249864	2.81329753	3.40657895	C
3.46296353	2.52575954	3.39062470	N
2.71174077	2.81137996	4.36891127	O
1.33386427	1.95891546	0.72733301	H

```
    1.69893724    2.50778938    1.62908742     C
    4.13562187    2.82158041    0.60799974     H
    5.13855957    4.35096326    3.24968196     C
    0.88918068    2.53804324    2.39189447     H
    6.20703337    4.62252388    3.38489059     H
    4.52979692    4.86567316    4.02594866     H
    1.92909480    3.55118545    1.31127791     H
    4.81201038    4.71669038    2.24840122     H

outcell: Unit cell vectors (Ang):
       10.280338    0.001932   -0.182257
        5.142390    8.888979   -0.248053
       -0.483819   -0.484797   31.385460
```

Nit8 w/o nitroxyl O on Cu step on-top

```
    7.96460173    0.01463733   -0.21618821     Cu
    6.70163256    2.26969434    0.18604050     Cu
    9.26668572    2.25406404   -0.22765170     Cu
    5.38920834    4.51974134   -0.05652150     Cu
    7.97341612    4.51391832   -0.11409710     Cu
   10.52725240    4.48523200   -0.30087285     Cu
    4.09520063    6.75496613   -0.09662224     Cu
    6.65769827    6.75601625   -0.20631152     Cu
    9.23742900    6.69069796   -0.28533631     Cu
   11.85340629    6.66168567   -0.30534461     Cu
    1.44799474    0.72150224   -2.07574013     Cu
    3.98770033    0.73030512   -2.25702220     Cu
    6.55041232    0.74260446   -2.21868916     Cu
    9.19628800    0.73258398   -2.30226594     Cu
    2.70838338    2.96662400   -2.13692800     Cu
    5.25833325    2.93094813   -2.09633269     Cu
    7.82315872    2.94481806   -2.20266364     Cu
   10.48741005    2.94931923   -2.35354103     Cu
    3.98571265    5.18970014   -2.14645984     Cu
    6.56479519    5.19969571   -2.25808546     Cu
    9.15557397    5.20637886   -2.37801934     Cu
   11.74947381    5.20077023   -2.42543852     Cu
    5.30444051    7.46434253   -2.25212307     Cu
    7.87716183    7.47204022   -2.32282676     Cu
   10.45167328    7.45808415   -2.38444516     Cu
   13.03450829    7.46950715   -2.36172276     Cu
    0.10704468    1.45077914   -4.33033386     Cu
    2.67033191    1.45802487   -4.35496224     Cu
    5.25696855    1.45359621   -4.39601033     Cu
    7.83203346    1.45340174   -4.44214171     Cu
    1.39565384    3.68705665   -4.40745931     Cu
    3.96849234    3.68643683   -4.32652888     Cu
    6.53901441    3.68160961   -4.37500638     Cu
    9.11339840    3.68225407   -4.45157117     Cu
    2.69613158    5.92933154   -4.39132403     Cu
    5.24409556    5.92216457   -4.41435598     Cu
    7.82155976    5.92241494   -4.47932717     Cu
   10.39988846    5.92084813   -4.59640402     Cu
    3.96582814    8.16421189   -4.36966139     Cu
```

```
    6.53654696    8.16643879   -4.41755253     Cu
    9.11631169    8.16767219   -4.52005152     Cu
   11.70814965    8.16554502   -4.49921893     Cu
    6.16543068    2.94706064    6.30264541     O
    4.92861257    1.08507454    7.44620498     H
    4.77919007    1.12773315    6.43656848     N
    4.39683749    3.11759735    4.15674840     H
    5.41079636    2.14148686    5.73410922     C
    6.87675834    4.36503519    4.35115100     H
    4.13282838    0.46574896    6.00861942     H
    5.81612681    4.65185879    2.91145035     H
    5.08076506    2.23688054    4.22539470     C
    3.20052787    3.04852568    2.02368335     H
    6.66501648    4.04637139    3.30474068     C
    3.32385776    0.91106985    3.83527672     H
    4.39628669    1.03016964    3.56074930     C
    3.36749176    2.10380513    1.45817449     C
    6.31368248    2.53418523    3.27507758     C
    2.42078546    1.51336785    1.45721689     H
    7.55633796    4.26516893    2.67104105     H
    7.95816149    2.07771799    4.68732275     H
    3.58760991    2.38015965    0.39995124     H
    4.57010786    1.30031220    2.03757464     C
    4.91952302    0.08254977    3.82957992     H
    7.57178367    1.71540763    3.70823569     C
    5.83396601    2.08992121    1.92002033     N
    7.34939084    0.62757117    3.79902112     H
    8.36792079    1.83067579    2.93852891     H
    4.70392326   -0.04218883    1.27372940     C
    3.75149471   -0.63631986    1.32222671     H
    5.53250066   -0.65544794    1.69544577     H
    4.93567272    0.15006227    0.20020389     H

outcell: Unit cell vectors (Ang):
       10.301547    0.000657   -0.163714
        5.155557    8.929215    0.084105
       -0.377809    0.566482   30.645425
```

Nit9 on flat Au(111) via NO hcp site

```
   -0.11861831    0.07126972   -0.21380613     Au
    2.80369370    0.06342311   -0.19420511     Au
    5.72407679    0.06480441   -0.19224954     Au
    1.34643222    2.59798931   -0.22184679     Au
    4.24582734    2.58402766   -0.29003401     Au
    7.21687535    2.57577998   -0.26872933     Au
    2.79300121    5.13102748   -0.27455281     Au
    5.72013047    5.13897985   -0.28378202     Au
    8.65320979    5.11745748   -0.22568024     Au
    1.37067844    0.88508603   -2.73422594     Au
    4.29288419    0.87496547   -2.73133789     Au
    7.22062878    0.87257509   -2.70758731     Au
    2.82617689    3.41138198   -2.76919519     Au
    5.75522014    3.40813277   -2.74431408     Au
    8.68680482    3.40597698   -2.72434023     Au
```

```
    4.28649213    5.94060756   -2.77493998     Au
    7.21538696    5.93500345   -2.75272340     Au
   10.13909576    5.93322414   -2.73934559     Au
   -0.05727943    1.69495238   -5.23028214     Au
    2.86589405    1.69227937   -5.21355640     Au
    5.79296564    1.69206995   -5.19816825     Au
    1.40246231    4.22250437   -5.25245676     Au
    4.32907156    4.21925009   -5.23449099     Au
    7.25213184    4.21643058   -5.21273301     Au
    2.86254338    6.74997193   -5.26283319     Au
    5.78775699    6.74826089   -5.23784572     Au
    8.71085559    6.74397119   -5.22307278     Au
   -0.02641267   -0.01545089   -7.73441234     Au
    2.89730632   -0.01818168   -7.71836365     Au
    5.82297605   -0.02286656   -7.69408149     Au
    1.43305823    2.50970507   -7.74722883     Au
    4.35589663    2.50602066   -7.72417241     Au
    7.28670366    2.50366146   -7.70334061     Au
    2.89201802    5.03856021   -7.75787841     Au
    5.81894812    5.03720551   -7.73685729     Au
    8.74547001    5.03279295   -7.71938728     Au
    4.55995644    1.11011575    4.27621640     H
    7.92812045    2.08167298    4.24149856     H
    3.85171591    1.89800380    3.93736487     C
    3.66087864    1.75604860    2.84887061     H
    8.12672539    3.14976503    3.99958588     C
    8.43264114    3.21408594    2.93107802     H
    2.88874341    1.77153516    4.48113681     H
    8.95454217    3.51889880    4.64204626     H
    5.95793317    2.92811492    8.11522027     H
    5.76743947    3.40667558    2.13774801     O
    5.72202559    3.47674291    3.42266168     N
    4.43236301    3.31751385    4.18343876     C
    6.86757959    4.02321949    4.23588396     C
    6.63819120    3.68750134    8.07314093     N
    4.95182147    3.52559475    5.59954062     C
    6.26736855    3.88513360    5.64393491     C
    7.23607339    3.83963267    8.88793931     H
    7.09899344    4.19311168    6.86504447     C
    4.28599869    3.41128317    6.47499388     H
    8.13113727    4.88706340    6.79791132     O
    3.42089963    4.41230022    3.73408964     C
    3.15868863    4.26056491    2.66160247     H
    7.13875694    5.50272068    3.83013039     C
    7.46142862    5.54447885    2.76471036     H
    2.48988709    4.36144740    4.34060953     H
    7.93070034    5.92856712    4.48243937     H
    3.85403302    5.43040710    3.84225512     H
    6.22205491    6.12398726    3.93691911     H

outcell: Unit cell vectors (Ang):
        8.775818   -0.008416    0.059533
        4.380415    7.580053   -0.036437
        0.197467   -0.259517   27.002498
```

Nit9 on flat Au(111) via NO fcc site

-0.13025692	0.04630903	-0.21891075	Au
2.78302323	0.05540902	-0.18237201	Au
5.71610889	0.01619816	-0.21626618	Au
1.32213152	2.58044860	-0.19031656	Au
4.23705807	2.59217088	-0.23370178	Au
7.19346574	2.59141967	-0.21436312	Au
2.79001423	5.10115303	-0.18552886	Au
5.71470379	5.11274489	-0.16574173	Au
8.63138033	5.11006792	-0.13061410	Au
1.35700409	0.87191405	-2.71571617	Au
4.27815366	0.87099860	-2.69170150	Au
7.20705758	0.86975536	-2.66399812	Au
2.81227187	3.40219428	-2.72082581	Au
5.74260260	3.40302649	-2.69141805	Au
8.67240444	3.40286166	-2.66485877	Au
4.28054007	5.92538105	-2.70900228	Au
7.20419889	5.92794205	-2.68096437	Au
10.12912117	5.91886038	-2.66366757	Au
-0.07420777	1.68295171	-5.21047656	Au
2.85153915	1.68284579	-5.18095161	Au
5.77561858	1.68434334	-5.15686063	Au
1.38921169	4.21270622	-5.21321849	Au
4.31337869	4.21322537	-5.17934187	Au
7.23590770	4.21269835	-5.15063721	Au
2.85192580	6.74099993	-5.20931501	Au
5.77474255	6.73973752	-5.17446571	Au
8.69805951	6.74110942	-5.15068737	Au
-0.03939485	-0.02993480	-7.71204805	Au
2.87949767	-0.03051370	-7.68262055	Au
5.80622956	-0.03057121	-7.65082279	Au
1.41844573	2.50108320	-7.71369269	Au
4.34063710	2.50165949	-7.68124378	Au
7.26890816	2.50023093	-7.65352687	Au
2.88008339	5.02817750	-7.71502579	Au
5.80472889	5.03078800	-7.68587571	Au
8.72848985	5.02788655	-7.65623161	Au
4.55394691	-0.77889887	4.28753118	H
7.89701275	0.20069539	4.25391161	H
3.84476400	0.00763724	3.94761894	C
3.67425819	-0.12281866	2.85371007	H
8.09799702	1.27099637	4.02387374	C
8.39982285	1.34729312	2.95480308	H
2.87371934	-0.13328620	4.47323002	H
8.92868063	1.63089686	4.66784025	H
5.93725360	1.03723906	8.15316130	H
5.72887280	1.59692787	2.16765996	O
5.69480817	1.61346331	3.45425063	N
4.40916149	1.43005933	4.21556076	C
6.84232413	2.14620851	4.27267215	C
6.61924889	1.79481922	8.10916904	N
4.92974674	1.62824152	5.63293944	C
6.24369404	1.99435090	5.67947553	C
7.21690979	1.94866388	8.92398108	H

```
    7.07822219    2.29945980    6.90002437     C
    4.26434569    1.50456097    6.50736451     H
    8.11196921    2.99110512    6.82992199     O
    3.38300401    2.51786630    3.78289349     C
    3.09390618    2.36195070    2.71837091     H
    7.11697517    3.62865870    3.88211157     C
    7.44707832    3.68001014    2.81946193     H
    2.46699405    2.46533750    4.41164448     H
    7.90410489    4.04758681    4.54440808     H
    3.81436039    3.53820659    3.87562960     H
    6.19901470    4.24780157    3.98934577     H

outcell: Unit cell vectors (Ang):
        8.772594   -0.000597    0.088127
        4.385121    7.584768   -0.002700
        0.280228   -0.198395   26.890750
```

Nit9 on flat Au(111) via >CO

```
   -0.12409249    0.04848578   -0.48277625     Au
    2.79237315    0.05826418   -0.47790262     Au
    5.71906941    0.04547001   -0.51756273     Au
    1.32865874    2.58308664   -0.48894062     Au
    4.22392964    2.59668736   -0.60273234     Au
    7.20317215    2.58491418   -0.54982185     Au
    2.78880688    5.11293731   -0.46765370     Au
    5.72320557    5.10668666   -0.51278678     Au
    8.64543308    5.10778723   -0.45246223     Au
    1.37087387    0.86631475   -3.00153495     Au
    4.29583913    0.86137074   -3.01931395     Au
    7.22249179    0.85967385   -2.99165461     Au
    2.82018093    3.40018715   -3.04472116     Au
    5.75775840    3.39103649   -3.03068180     Au
    8.68531699    3.38950799   -2.99518647     Au
    4.28853240    5.91188650   -3.02301485     Au
    7.21935536    5.91146723   -3.00217220     Au
   10.14195597    5.90469686   -2.99299179     Au
   -0.04453384    1.67101679   -5.49737157     Au
    2.87966531    1.67040605   -5.49548362     Au
    5.80597244    1.66847846   -5.49787408     Au
    1.41187614    4.19710736   -5.51236205     Au
    4.33868147    4.19718787   -5.51033562     Au
    7.26318454    4.19349200   -5.48524235     Au
    2.87572115    6.71783181   -5.51364210     Au
    5.80204445    6.71941697   -5.48468143     Au
    8.72281382    6.71531869   -5.48445857     Au
   -0.00377420   -0.04056555   -8.01050119     Au
    2.91587457   -0.04376398   -8.00559390     Au
    5.84368456   -0.04928264   -7.98998948     Au
    1.45330479    2.48410300   -8.02505117     Au
    4.37342434    2.48202304   -8.01555584     Au
    7.30767631    2.48024382   -7.99216845     Au
    2.91173821    5.00673288   -8.03636122     Au
    5.83743618    5.01144789   -8.01395253     Au
    8.76304279    5.00397401   -8.00354124     Au
```

```
    2.61272703    1.93777709    4.06411551     H
    2.99878519    2.80822307    3.48869200     C
    3.10044024    2.51668902    2.41952386     H
    2.25219075    3.63093724    3.55869868     H
    3.89756593    1.55786873    7.29586656     H
    6.49353686   -0.32065836    4.07897635     H
    6.43955740    0.16731759    3.18332358     N
    6.71302564   -0.33057802    2.32673046     H
    4.54480897    2.39686525    7.63379812     C
    5.85603502    1.39896110    3.00900367     C
    5.69980707    1.89026389    1.86610879     O
    4.35780782    3.30100520    4.05523866     C
    3.91254174    3.13448407    8.17589759     H
    5.40719938    2.18518014    4.20710568     C
    4.18936224    3.69012699    5.50915997     N
    3.45823698    4.68803549    5.87114042     O
    5.30443543    1.99218142    8.34023426     H
    5.88621964    2.10045893    5.47953764     C
    5.23176954    3.09227716    6.42653249     C
    6.68092038    1.41284861    5.82368618     H
    4.86748354    4.53028067    3.24687292     C
    4.12089727    5.35185671    3.32725005     H
    4.99953963    4.26382837    2.17619017     H
    6.20805953    4.20258767    6.91135619     C
    5.83791730    4.90969002    3.63561422     H
    5.64688227    4.94529712    7.52078969     H
    7.02440456    3.76901833    7.53112403     H
    6.66787485    4.73454291    6.05002819     H

outcell: Unit cell vectors (Ang):
        8.773175   -0.005172    0.044891
        4.381601    7.569409   -0.015966
        0.132408   -0.159147   28.424845
```

Nit9 on flat Au(111) parallel

```
   -0.13377867    0.04666364   -0.58154928     Au
    2.79106510    0.05474511   -0.58466838     Au
    5.72174163    0.05638710   -0.53080016     Au
    1.32973648    2.57472960   -0.61644901     Au
    4.26449040    2.57855191   -0.57485134     Au
    7.18439974    2.58409936   -0.50708441     Au
    2.80004552    5.10147630   -0.58189635     Au
    5.72633519    5.10572161   -0.54737992     Au
    8.65171746    5.10511920   -0.54033605     Au
    1.35596996    0.86872582   -3.09847533     Au
    4.28520784    0.87390736   -3.06355816     Au
    7.21112549    0.87918381   -3.01080571     Au
    2.82476975    3.39784832   -3.09297812     Au
    5.75257257    3.40100975   -3.05349175     Au
    8.67267134    3.40347990   -3.02238980     Au
    4.29001892    5.92415552   -3.07662742     Au
    7.21448283    5.92632042   -3.05441292     Au
   10.14452400    5.93087005   -3.00939755     Au
   -0.08625258    1.67163279   -5.58628049     Au
```

```
    2.84098135    1.67664181   -5.55111846     Au
    5.76739641    1.67979787   -5.50964082     Au
    1.38255358    4.19855095   -5.58382290     Au
    4.30603580    4.20387329   -5.54135879     Au
    7.23210744    4.20718140   -5.51056388     Au
    2.84754335    6.72432499   -5.57304135     Au
    5.77220402    6.72738139   -5.53970353     Au
    8.69830487    6.73309198   -5.50519529     Au
   -0.05874608   -0.03600867   -8.08033767     Au
    2.86653248   -0.03359189   -8.04551602     Au
    5.79455927   -0.02788901   -8.00561695     Au
    1.40776645    2.48897807   -8.07756696     Au
    4.33342697    2.49469257   -8.03971121     Au
    7.25864724    2.49730539   -8.00279615     Au
    2.87389593    5.01578359   -8.07283309     Au
    5.79887703    5.01867155   -8.03639677     Au
    8.72528292    5.02460951   -7.99876627     Au
    3.46537105    2.51306328    6.43613087     H
    4.68948210   -0.62876970    6.43325902     H
    2.89058399    2.81239023    5.53194143     C
    1.81571065    2.59113293    5.71852261     H
    4.53835862   -1.22865023    5.50855772     C
    3.64830975   -1.88160907    5.65199008     H
    3.00932193    3.90773037    5.37557161     H
    5.43574407   -1.86403137    5.34773486     H
    7.55742031    2.15384040    4.78006230     H
    1.92842623    0.06109977    4.61520131     O
    3.10911924    0.55667269    4.47373261     N
    3.36739358    2.02951073    4.27773460     C
    4.32427568   -0.31775475    4.27001553     C
    7.81910274    1.29521446    4.29236892     N
    4.88135971    2.01464749    4.11924434     C
    5.41248851    0.75885320    4.12072912     C
    8.79620787    0.96707374    4.36614920     H
    6.86404655    0.34760083    3.97416393     C
    5.43965801    2.96006950    3.98039776     H
    7.17119660   -0.79905691    3.58752078     O
    2.65727192    2.54165927    2.99270615     C
    1.55436330    2.41403852    3.07322244     H
    4.12614029   -1.17344987    2.98782663     C
    3.22615182   -1.81970666    3.10321320     H
    2.87847654    3.62068925    2.82859830     H
    5.02801112   -1.79511358    2.80581573     H
    3.00125587    1.97386746    2.10030698     H
    3.97198530   -0.52481317    2.09748769     H

outcell: Unit cell vectors (Ang):
        8.776873    0.012234    0.115518
        4.398162    7.578911    0.014144
        0.348978   -0.175655   28.413748
```

Nit9 on flat Cu(111) via NO fcc site

```
   -0.05036967   -0.01171124   -0.00167635     Cu
    2.56791115    0.00316743    0.07041685     Cu
```

5.18840744	0.01572112	0.10515870	Cu
7.81071501	0.04893684	0.13597004	Cu
1.28282281	2.25497142	0.06440827	Cu
3.89596451	2.25923493	0.10640158	Cu
6.51621550	2.27715978	0.13640470	Cu
9.13222553	2.31535467	0.16386416	Cu
2.60822398	4.49942364	0.12111647	Cu
5.22300746	4.51377147	0.14972983	Cu
7.83793817	4.53917276	0.19038883	Cu
10.46334675	4.56588240	0.22515823	Cu
3.93300784	6.75542496	0.14040311	Cu
6.55470526	6.77198051	0.17713154	Cu
9.16998509	6.79141212	0.22611501	Cu
11.79660040	6.81680523	0.25716063	Cu
1.31396379	0.76337764	-2.08726821	Cu
3.92853494	0.75542126	-2.04515864	Cu
6.53671355	0.77294486	-2.01272787	Cu
9.16898151	0.82892699	-1.98291900	Cu
2.64880648	3.01511756	-2.06559900	Cu
5.23117598	3.01952901	-2.04044650	Cu
7.82458639	3.04775386	-1.99988097	Cu
10.48262454	3.06364429	-1.93956283	Cu
3.95873573	5.24853324	-2.03040037	Cu
6.53408011	5.26264497	-1.99716878	Cu
9.16667543	5.27781578	-1.92636889	Cu
11.80035848	5.30443874	-1.88778774	Cu
5.28506129	7.49770111	-2.00788743	Cu
7.88860307	7.54316109	-1.93003413	Cu
10.51509034	7.53092934	-1.90017421	Cu
13.15401685	7.58791456	-1.85600162	Cu
0.01253961	1.49066780	-4.25860159	Cu
2.62464796	1.48675298	-4.21114562	Cu
5.24939355	1.49230125	-4.16551272	Cu
7.87572578	1.53601447	-4.14024584	Cu
1.32067044	3.74377716	-4.20149353	Cu
3.88315352	3.72180774	-4.21587746	Cu
6.60884874	3.74455945	-4.17241644	Cu
9.20563275	3.80487447	-4.09254520	Cu
2.62512740	6.02947542	-4.10442292	Cu
5.26482977	6.09077834	-4.19017401	Cu
7.92192391	6.05754746	-4.03104672	Cu
10.52365721	6.05705665	-4.06237930	Cu
3.98533933	8.28369612	-4.13837699	Cu
6.62369486	8.29760218	-4.10370490	Cu
9.23873783	8.29455353	-4.06556099	Cu
11.85639976	8.32423744	-4.03324457	Cu
3.36839102	6.68621195	-7.91236391	H
7.09282174	6.77844925	-7.71503739	H
2.94444032	5.68074791	-7.69857806	C
2.56777690	5.67799745	-6.64608345	H
2.06963337	5.50523135	-8.36574286	H
7.55885794	5.77845581	-7.57324602	C
5.45311333	5.55816777	-11.74857892	H
7.93068402	5.71720865	-6.51999472	H
5.25378839	4.94712257	-7.09443269	N
4.02603083	4.58149777	-7.89339284	C

```
    8.43574267    5.67770677   -8.24955526     H
    5.24201771    4.59029505   -5.71961939     O
    4.62207635    4.62325871   -9.29342412     C
    6.32993914    5.03953575  -11.69921270     N
    5.98077869    4.68344640   -9.28816378     C
    3.97701112    4.55472590  -10.18941384     H
    6.53125872    4.64837301   -7.85001660     C
    6.96129942    5.08359307  -12.50131291     H
    6.89738591    4.66784981  -10.48675745     C
    8.08583538    4.30635023  -10.40835740     O
    3.42416295    3.17343878   -7.61328196     C
    3.04341814    3.10381934   -6.56540838     H
    2.56084506    2.98760353   -8.29129914     H
    7.16352411    3.25799211   -7.55576777     C
    7.53956050    3.20643715   -6.50491795     H
    8.02205387    3.10031129   -8.24349815     H
    4.16705225    2.36161803   -7.76452127     H
    6.43636247    2.43035216   -7.70043703     H

outcell: Unit cell vectors (Ang):
       10.480729    0.087782    0.143034
        5.316197    9.031723    0.144728
        0.320981    0.191472   25.331454
```

Nit9 on flat Cu(111) via NO hcp site

```
    0.05608974    0.03109783    0.02901606     Cu
    2.68032404    0.05325529    0.03588010     Cu
    5.30093486    0.08752769    0.03339151     Cu
    7.92140394    0.11252720    0.02196063     Cu
    1.39308914    2.28816244    0.03406341     Cu
    4.01921010    2.32168062    0.03456380     Cu
    6.63634646    2.34563747    0.02595575     Cu
    9.25725090    2.36746772    0.00749737     Cu
    2.73004302    4.54985622    0.01998513     Cu
    5.34733862    4.57545077    0.01736713     Cu
    7.96958732    4.60060543    0.00952691     Cu
   10.59466207    4.63430711    0.00240820     Cu
    4.05812223    6.80985042   -0.00064286     Cu
    6.68092274    6.83318985   -0.00209877     Cu
    9.30119932    6.86015158    0.00686796     Cu
   11.92507145    6.88707464   -0.00434280     Cu
    1.36047452    0.78966719   -2.10497315     Cu
    3.97991644    0.82814405   -2.11096985     Cu
    6.60007154    0.85483079   -2.12313094     Cu
    9.22687757    0.87588353   -2.12487113     Cu
    2.69151855    3.04365328   -2.10271805     Cu
    5.32636597    3.08508448   -2.13628158     Cu
    7.93312713    3.10858501   -2.13709977     Cu
   10.56776563    3.12571717   -2.12056887     Cu
    4.03881176    5.31882301   -2.14414127     Cu
    6.65419448    5.32951572   -2.16929850     Cu
    9.26327253    5.37274932   -2.14822122     Cu
   11.90159653    5.38450728   -2.13505759     Cu
    5.35954628    7.55643717   -2.15883741     Cu
```

```
    7.98441631    7.58506460   -2.16058927     Cu
   10.60763508    7.63016190   -2.15233491     Cu
   13.21726730    7.65911890   -2.15600791     Cu
   -0.01503191    1.48967402   -4.27385931     Cu
    2.60716207    1.52949067   -4.26658980     Cu
    5.23027511    1.54733896   -4.27287646     Cu
    7.86155527    1.55860304   -4.28160991     Cu
    1.33026530    3.74716286   -4.27034239     Cu
    3.93128085    3.77318768   -4.21872114     Cu
    6.59330471    3.74961281   -4.32602392     Cu
    9.23186100    3.80797783   -4.22640009     Cu
    2.65649952    6.01363767   -4.27470355     Cu
    5.26158572    6.06988539   -4.32409916     Cu
    7.98916147    6.11339479   -4.31601059     Cu
   10.57262996    6.09051554   -4.27199462     Cu
    3.97912049    8.28482617   -4.29474863     Cu
    6.61002584    8.33647500   -4.27680404     Cu
    9.25252872    8.36076470   -4.28753883     Cu
   11.85586155    8.35322095   -4.32193423     Cu
    4.80579110    7.51078704   -8.07400509     H
    8.58357151    7.61505521   -7.93262747     H
    4.40241474    6.50265561   -7.83423741     C
    4.05098081    6.51692708   -6.77377468     H
    3.51616070    6.29913955   -8.47728118     H
    9.03862376    6.61533852   -7.75641050     C
    6.95012910    6.40595891  -11.89321829     H
    9.41027299    6.58717481   -6.70315445     H
    6.72382653    5.81340093   -7.23757159     N
    5.49604607    5.41461373   -8.02301625     C
    9.91140412    6.48080113   -8.43213325     H
    6.70521934    5.43839934   -5.86715466     O
    6.08335393    5.43516175   -9.42884831     C
    7.82303504    5.88156157  -11.83684655     N
    7.44267060    5.50043479   -9.42982299     C
    5.43506815    5.36069404  -10.32192246     H
    7.99844778    5.48863602   -7.99390839     C
    8.46942318    5.93661385  -12.62664208     H
    8.36908957    5.48844453  -10.62234211     C
    9.55495363    5.11830421  -10.53598145     O
    4.91283012    4.01099968   -7.68655857     C
    4.58659221    3.97039634   -6.61810503     H
    4.01770233    3.80650280   -8.31516899     H
    8.62454615    4.10165684   -7.67220549     C
    9.01540684    4.07683452   -6.62449591     H
    9.47341131    3.92016860   -8.36657220     H
    5.64828982    3.19460213   -7.84933637     H
    7.89189594    3.27399672   -7.78363152     H

outcell: Unit cell vectors (Ang):
       10.490816    0.104354   -0.012029
        5.335862    9.033811   -0.043308
       -0.037686   -0.105715   25.380573
```

Nit9 on flat Cu(111) via >CO

0.05921928	0.03321481	-0.04507002	Cu
2.70468695	0.07879649	-0.01366395	Cu
5.33880685	0.12088001	-0.02031742	Cu
7.97291443	0.15830532	-0.05081755	Cu
1.41935129	2.29091262	-0.02175761	Cu
4.05662437	2.33417870	-0.01081464	Cu
6.69276372	2.37506246	-0.02501369	Cu
9.32947974	2.41015167	-0.05228354	Cu
2.77602783	4.54948288	-0.03664785	Cu
5.40923352	4.58975266	-0.01714277	Cu
8.04879088	4.63099602	-0.01989709	Cu
10.69189505	4.67778697	-0.04347705	Cu
4.12773046	6.80633202	-0.06151152	Cu
6.76624947	6.84998944	-0.03228873	Cu
9.40440838	6.89195140	-0.03166465	Cu
12.04225807	6.93289667	-0.06155252	Cu
1.37148984	0.79830587	-2.16681469	Cu
4.00752399	0.84037657	-2.16285721	Cu
6.64482744	0.87655586	-2.18178014	Cu
9.28661747	0.91160552	-2.19581406	Cu
2.72467924	3.04791311	-2.16712963	Cu
5.35943796	3.09354885	-2.16105495	Cu
8.00159603	3.13293701	-2.16476416	Cu
10.64825437	3.16643410	-2.17955706	Cu
4.08617064	5.30639482	-2.18754862	Cu
6.72119480	5.34781458	-2.16622744	Cu
9.36231596	5.38603934	-2.15831758	Cu
12.00037151	5.42667433	-2.19185479	Cu
5.43812523	7.55478994	-2.20222165	Cu
8.07275158	7.61511089	-2.16871842	Cu
10.71255958	7.65055354	-2.19372003	Cu
13.34769714	7.68656991	-2.21894211	Cu
-0.00932842	1.47965641	-4.33462647	Cu
2.62980900	1.52657045	-4.31617510	Cu
5.26834618	1.56500395	-4.31062042	Cu
7.91398312	1.59182528	-4.32401092	Cu
1.34890279	3.73491855	-4.32744778	Cu
3.98042063	3.77737156	-4.30406484	Cu
6.64213587	3.78797562	-4.26962867	Cu
9.27355689	3.84913584	-4.28257584	Cu
2.70848637	5.98673754	-4.34949484	Cu
5.34467419	6.03303146	-4.32688306	Cu
8.04920541	6.11256285	-4.25150163	Cu
10.63770977	6.11397264	-4.32082303	Cu
4.05732407	8.24385713	-4.36494113	Cu
6.69439025	8.30903936	-4.31488811	Cu
9.33888965	8.34742641	-4.32662844	Cu
11.97321503	8.37080065	-4.36379056	Cu
6.64497578	3.94293471	-12.01553739	H
7.53486544	2.53823219	-8.71975607	H
7.24172664	4.84603855	-12.26996498	C
8.09457482	4.53594742	-12.91344959	H
6.59840289	5.54457950	-12.85175757	H
8.29992131	3.14306941	-8.18422906	C

```
    4.31321168    5.56694010   -8.55354212     H
    9.29353993    2.66506816   -8.33331170     H
    8.65291987    4.59091338  -10.20191553     N
    7.78775151    5.54452458  -10.99529929     C
    8.06800973    3.13795299   -7.09489559     H
    9.77117731    4.15627444  -10.66405736     O
    6.70789936    5.83243535   -9.96635690     C
    4.78568806    5.62329767   -7.65116442     N
    6.98427920    5.30633975   -8.73781745     C
    5.81391210    6.43071329  -10.22152512     H
    8.35022687    4.59818461   -8.71446428     C
    4.22716544    5.71974979   -6.78585439     H
    6.13102815    5.43328887   -7.51146465     C
    6.66093733    5.37739890   -6.36070133     O
    8.61687356    6.80205248  -11.38964145     C
    9.48890034    6.47457431  -11.99932072     H
    8.00539272    7.51525646  -11.98615079     H
    9.45433249    5.40480026   -7.96859050     C
   10.43233297    4.89297849   -8.11575062     H
    9.23550470    5.46249569   -6.87859018     H
    8.99968633    7.33268905  -10.49145459     H
    9.53938530    6.44311009   -8.35617964     H

outcell: Unit cell vectors (Ang):
       10.551914    0.165180   -0.013520
        5.419387    9.028534   -0.032673
       -0.041395   -0.069368   26.332497
```

Nit9 on Cu adatom on-top via NO

```
    5.27162100    3.11358575    2.07250430     Cu
   -0.01581020   -0.03227689    0.07041151     Cu
    2.60067461    0.04915234    0.13254366     Cu
    5.22350790    0.13204996    0.15882923     Cu
    7.81409183    0.13072338    0.15368477     Cu
    1.36486442    2.27295312    0.06053577     Cu
    3.96627198    2.33842723    0.11891760     Cu
    6.61555489    2.39667660    0.09169877     Cu
    9.20012363    2.44663512    0.13809787     Cu
    2.71686307    4.55863858    0.12228838     Cu
    5.33178327    4.65063929    0.11947795     Cu
    7.94485530    4.71106874    0.15260362     Cu
   10.54490789    4.74255073    0.17721904     Cu
    4.02267462    6.84638296    0.07936709     Cu
    6.63590539    6.92687157    0.15999105     Cu
    9.25115014    7.00816420    0.19474735     Cu
   11.84346821    7.02219986    0.18777862     Cu
    1.26503616    0.77759045   -2.03352648     Cu
    3.89455335    0.86276250   -1.99972443     Cu
    6.50916517    0.87851467   -2.00758756     Cu
    9.09186731    0.92861166   -1.95804518     Cu
    2.67214895    3.07817729   -2.04782779     Cu
    5.28769981    3.13561946   -2.04947753     Cu
    7.89252232    3.21114488   -2.01271952     Cu
   10.49000615    3.25435227   -1.96069901     Cu
```

```
     4.00903869    5.34679986   -2.03943706     Cu
     6.62335875    5.44466927   -1.99132142     Cu
     9.23489846    5.51667763   -1.94917532     Cu
    11.84302666    5.52403896   -1.92813961     Cu
     5.31120272    7.64359433   -2.01750013     Cu
     7.92158930    7.73826753   -1.96472152     Cu
    10.53140977    7.78922321   -1.94182796     Cu
    13.13705915    7.79696587   -1.93437016     Cu
    -0.05677137    1.51676085   -4.20821804     Cu
     2.55830033    1.55075595   -4.16204109     Cu
     5.17653920    1.60025632   -4.13938444     Cu
     7.77824070    1.66658325   -4.11802566     Cu
     1.35599721    3.80239035   -4.21304318     Cu
     3.96444794    3.84796932   -4.16981052     Cu
     6.57753719    3.93498701   -4.14141977     Cu
     9.18145939    4.00815396   -4.10580462     Cu
     2.70558337    6.08706254   -4.20682680     Cu
     5.30673690    6.15330425   -4.15939418     Cu
     7.91877884    6.23901284   -4.10137184     Cu
    10.52979446    6.26469896   -4.08434458     Cu
     3.99953629    8.37792308   -4.19723837     Cu
     6.59891388    8.44846987   -4.11748472     Cu
     9.22231451    8.49054742   -4.09508005     Cu
    11.83131466    8.53201140   -4.09672012     Cu
     6.12954625    1.34341310    6.79398198     H
     5.46024566    0.92266867    6.01131070     C
     4.91721491    0.05249200    6.44129517     H
     6.09140245    0.56701563    5.16669018     H
     6.46845716    4.97171825    6.66056691     H
     3.23788459    3.54666765    9.23588138     H
     4.45396528    1.99774391    5.51721829     C
     3.09702449    2.04546042    7.37474671     H
     3.69537346    2.64762859    6.66629031     C
     5.20718905    3.19393867    5.01119133     N
     5.80721462    5.45596118    5.90827564     C
     5.94892164    3.12128852    3.91313730     O
     2.86392792    4.43792858    8.91013103     N
     3.82080788    4.00319958    6.68513218     C
     2.92404084    0.55344640    4.84358447     H
     3.49001211    1.42063868    4.43733235     C
     6.41921540    5.72071981    5.01838729     H
     4.65326788    4.50664136    5.49349116     C
     2.51907827    5.09734532    9.61058386     H
     4.06202367    1.07704435    3.54359354     H
     3.20935449    4.96653521    7.67240314     C
     5.37997860    6.38386036    6.34637494     H
     3.00683718    6.16065775    7.38840376     O
     2.75141556    2.18164439    4.10285521     H
     3.76044863    5.16803655    4.40290144     C
     4.38003600    5.46713730    3.52575121     H
     2.97752175    4.46471278    4.04420469     H
     3.26148695    6.06413917    4.82952262     H

outcell: Unit cell vectors (Ang):
       10.423804    0.214541    0.141065
        5.396619    9.172974    0.014768
```

0.351358 -0.171974 27.172766

Nit9 on Cu adatom on-top via >CO

5.65068747	3.21617669	2.00868530	Cu
0.00376423	0.06789041	0.03439320	Cu
2.67178857	0.08590149	0.05186516	Cu
5.32603050	0.09001110	0.08221675	Cu
7.98802059	0.09588446	0.07702040	Cu
1.35158207	2.29066725	0.08327089	Cu
4.02745930	2.31089991	0.14677692	Cu
6.69687774	2.28279882	0.02185739	Cu
9.32449717	2.33033771	0.13488746	Cu
2.69038020	4.51437077	0.11077104	Cu
5.34368443	4.55318037	0.02318843	Cu
7.96315871	4.50883250	0.22814542	Cu
10.65998793	4.55173950	0.19321946	Cu
4.02938684	6.73785907	0.09684700	Cu
6.69183398	6.75273509	0.12400188	Cu
9.33872038	6.75697463	0.16402293	Cu
12.00799227	6.77657473	0.17960278	Cu
1.36562670	0.75536801	-2.07794799	Cu
4.03389385	0.77390106	-2.06698912	Cu
6.68613309	0.77665270	-2.08347331	Cu
9.34466499	0.79540429	-2.03111143	Cu
2.71762286	2.97323089	-2.02656252	Cu
5.36294708	2.98553802	-2.10129415	Cu
8.03143465	3.00598121	-2.04282391	Cu
10.69043278	3.01503801	-1.95742753	Cu
4.04636118	5.19968760	-2.07083633	Cu
6.71687499	5.20965797	-2.04551753	Cu
9.36349838	5.21618595	-1.93781170	Cu
12.02869288	5.23564236	-1.93244132	Cu
5.39146601	7.41535954	-2.02887022	Cu
8.05254745	7.43689418	-1.99507443	Cu
10.70868278	7.45088563	-1.96432985	Cu
13.36688236	7.46026942	-1.96353909	Cu
0.03564914	1.44937441	-4.20478065	Cu
2.69154270	1.45999505	-4.19446681	Cu
5.35234350	1.47094427	-4.23112864	Cu
8.01757917	1.48545562	-4.20996103	Cu
1.37455162	3.67238120	-4.15814108	Cu
4.03060742	3.68453388	-4.20481898	Cu
6.69852266	3.69936658	-4.19894839	Cu
9.35997534	3.71722506	-4.11375232	Cu
2.70915327	5.89481336	-4.17360261	Cu
5.37694348	5.91315986	-4.19658342	Cu
8.04427073	5.92556097	-4.12647611	Cu
10.69582470	5.93189124	-4.08644588	Cu
4.05653643	8.11622749	-4.16509103	Cu
6.71987017	8.13123769	-4.13709345	Cu
9.37727373	8.14189873	-4.11205321	Cu
12.03840376	8.15257887	-4.12005853	Cu
4.99748550	2.69322239	9.75238400	H

```
    3.90308433    2.50732098    9.68712102     C
    3.36746667    3.38051749   10.12201009     H
    3.66388450    1.60583041   10.29380335     H
    6.81823446    1.26560690    7.01253439     H
    5.50118275    5.36304850    6.07972974     H
    3.45970261    2.26490589    8.22021061     C
    3.70127971    4.40232693    7.40198613     H
    3.94620580    3.33435345    7.25274127     C
    4.17445677    1.05936309    7.66086262     N
    6.19576494    0.75382003    6.24497619     C
    3.96538223   -0.12413989    8.12122102     O
    5.52262012    4.89195198    5.17551287     N
    4.65301321    2.81720021    6.20297042     C
    1.35618647    2.87187254    8.57988115     H
    1.92420725    2.02134800    8.14400855     C
    6.18724168   -0.33500702    6.47218023     H
    4.74226283    1.28572171    6.27819014     C
    5.91670895    5.38470683    4.36887297     H
    1.68931696    1.09407863    8.71372097     H
    5.24234912    3.55723464    5.04835426     C
    6.64446432    0.92030443    5.24276896     H
    5.46653401    2.92881677    3.96954160     O
    1.59385012    1.87675279    7.09267495     H
    3.84712798    0.56493627    5.22906226     C
    3.82909559   -0.52251349    5.46624124     H
    2.80351739    0.94683180    5.26544646     H
    4.23301978    0.72327557    4.19977919     H

outcell: Unit cell vectors (Ang):
       10.640449    0.053725    0.084388
        5.364790    8.891676    0.097394
        0.202677    0.165895   27.274091
```

Nit9 on Cu adatom on-top via -NH_2

```
    5.17587696    2.93072271    1.92890971     Cu
    0.04807401    0.02261897    0.04450492     Cu
    2.64243262    0.01932344    0.01415617     Cu
    5.23925737    0.03195757    0.01037861     Cu
    7.83727235    0.02383881   -0.04063248     Cu
    1.34190953    2.27223662    0.01633575     Cu
    3.91438863    2.25683747   -0.05509986     Cu
    6.54405351    2.26507333   -0.04065337     Cu
    9.13258294    2.27224663   -0.06333529     Cu
    2.64716430    4.50919711    0.02673638     Cu
    5.23971975    4.51872924   -0.02251788     Cu
    7.83594902    4.51342589   -0.03732009     Cu
   10.43465416    4.51234153   -0.06160249     Cu
    3.94196095    6.75986710   -0.01834131     Cu
    6.53630939    6.75949771   -0.04346141     Cu
    9.13489857    6.76302858   -0.05697097     Cu
   11.73302707    6.76288621   -0.08813436     Cu
    1.29126295    0.73587971   -2.13666470     Cu
    3.88499136    0.73606369   -2.18864292     Cu
    6.47670177    0.74221005   -2.20696421     Cu
    9.07691511    0.73973374   -2.21933152     Cu
```

2.58822463	2.98181275	-2.18292187	Cu
5.18583616	2.98328806	-2.24660121	Cu
7.77401159	2.98596153	-2.23038158	Cu
10.37487157	2.98688077	-2.23751019	Cu
3.89335680	5.21860562	-2.18997046	Cu
6.48505596	5.22120851	-2.21885049	Cu
9.08170931	5.22828569	-2.20843711	Cu
11.68316964	5.22562887	-2.23625212	Cu
5.18807501	7.47180372	-2.19546967	Cu
7.78464608	7.47159843	-2.21519490	Cu
10.37777613	7.48275760	-2.22745682	Cu
12.97449800	7.47532851	-2.27272668	Cu
-0.01910534	1.47839590	-4.27674619	Cu
2.57166454	1.47374013	-4.33904666	Cu
5.17019770	1.47196201	-4.38527116	Cu
7.77086725	1.47568541	-4.37863147	Cu
1.27506350	3.72446226	-4.30322659	Cu
3.86914580	3.72375286	-4.37915444	Cu
6.47408100	3.72556618	-4.41597481	Cu
9.06986426	3.72565415	-4.38568171	Cu
2.57559281	5.97354152	-4.32020584	Cu
5.17371199	5.97324178	-4.36241487	Cu
7.77232443	5.97196094	-4.37689643	Cu
10.36622973	5.97025916	-4.39401955	Cu
3.87241494	8.21572875	-4.33890564	Cu
6.47268153	8.21532628	-4.36571655	Cu
9.06479064	8.21283781	-4.39843462	Cu
11.66451495	8.21342923	-4.42347195	Cu
0.45039005	4.01650461	5.51252084	H
-0.04159244	3.26244907	4.85910379	C
-0.27950030	3.73653409	3.87960833	H
-0.99094120	2.94385987	5.34730823	H
2.95694390	2.50471182	7.76054219	H
4.62742195	3.98760020	4.20616765	H
0.86473582	2.01862020	4.64944629	C
2.43969448	2.92858688	3.23573232	H
2.26602064	2.37257203	4.17926043	C
1.18423639	1.37850545	5.98394816	N
3.13673551	1.42621367	7.55627607	C
0.27667279	0.80701019	6.69274078	O
5.17491831	3.13232719	4.01775702	N
3.24003549	1.86304492	4.99438100	C
-0.09583481	1.44215600	2.73774169	H
0.16297960	0.98540863	3.72059536	C
2.58105242	0.83108639	8.31466478	H
2.64869454	1.02686859	6.14111658	C
6.16885566	3.29213455	4.25341458	H
-0.76777820	0.63062112	4.21858079	H
4.71516751	1.98693673	4.80826778	C
4.22300274	1.21393916	7.66119534	H
5.54671726	1.19946608	5.26670902	O
0.81709374	0.10878439	3.51905915	H
2.84418253	-0.49885821	5.91319998	C
2.29665262	-1.05601711	6.70604571	H
2.43896883	-0.80411356	4.92455708	H
3.92473976	-0.75400083	5.94762674	H

```
outcell: Unit cell vectors (Ang):
       10.384455   -0.000774   -0.111152
        5.190884    8.987165   -0.081269
       -0.300301   -0.087654   27.646942
```

Nit9 on Cu step on-top via NO

```
    7.96475224    0.10720942   -0.14349343     Cu
    6.57315828    2.31539221    0.01142566     Cu
    9.23463444    2.35320133   -0.16825667     Cu
    5.33612269    4.61369524   -0.11749129     Cu
    7.92288885    4.60612118   -0.08163257     Cu
   10.48979914    4.60321519   -0.20766028     Cu
    4.06454434    6.82268493   -0.10039378     Cu
    6.63892538    6.83408768   -0.15368293     Cu
    9.21894712    6.83074372   -0.20973915     Cu
   11.81291262    6.80771248   -0.26732208     Cu
    1.43797063    0.82360631   -1.84919825     Cu
    4.02108008    0.82381777   -1.89001220     Cu
    6.57173558    0.83147674   -2.14417838     Cu
    9.19325790    0.82900390   -2.24733414     Cu
    2.73393766    3.06008718   -1.90245355     Cu
    5.27387067    3.03375729   -2.11231841     Cu
    7.86481912    3.05353820   -2.21275415     Cu
   10.50452774    3.04179854   -2.25489588     Cu
    3.99835787    5.27947610   -2.18202504     Cu
    6.59340766    5.29777572   -2.25817798     Cu
    9.17180460    5.29435748   -2.31145272     Cu
   11.76817147    5.27782308   -2.33149572     Cu
    5.31242733    7.55096332   -2.23428798     Cu
    7.88686217    7.57378140   -2.26932105     Cu
   10.46035482    7.54946543   -2.33107887     Cu
   13.04100429    7.52641029   -2.40404123     Cu
    0.13579860    1.54354912   -4.21236724     Cu
    2.70059425    1.54555358   -4.05824367     Cu
    5.26089033    1.54426807   -4.26939681     Cu
    7.84899225    1.55110596   -4.39813452     Cu
    1.42512631    3.76914302   -4.25367952     Cu
    3.97811455    3.76742169   -4.27736705     Cu
    6.55892023    3.77610334   -4.37978042     Cu
    9.14452222    3.77693178   -4.43388573     Cu
    2.70194884    6.01056208   -4.36815156     Cu
    5.27279959    6.01286042   -4.40450638     Cu
    7.85517285    6.01612269   -4.44894135     Cu
   10.43427303    6.01280164   -4.50375425     Cu
    3.98772458    8.24274919   -4.40821112     Cu
    6.56704757    8.25477179   -4.40964247     Cu
    9.14179350    8.25690723   -4.45252684     Cu
   11.72269863    8.25048342   -4.53103696     Cu
    8.30998635   -0.51985084    4.44676302     H
    8.53219830    1.25948023    4.68860107     H
    8.11861165    0.48408699    4.00706679     C
    8.65417258    0.54996175    3.03284001     H
```

```
    6.59824285    0.69994755    3.77310880     C
    6.18485123   -1.42981754    3.31542166     H
    5.79165502    0.07024676    5.82810649     H
    5.79562876    0.86075834    5.05538550     C
    6.01167924   -0.42539798    2.86976375     C
    5.19392317    1.42310818    7.67847485     H
    6.51561108   -0.40768179    1.86999752     H
    6.36389986    2.04848268    3.16841590     N
    6.99195459    2.44478536    2.08143729     O
    6.61968533    4.31445955    4.72565494     H
    4.32887256    1.90458091    7.43221329     N
    5.07274295    2.01588688    5.09020645     C
    4.91946879   -0.29546574    2.70505013     H
    5.72720661    4.29528416    4.06113162     C
    5.25722478    2.83910930    3.80265160     C
    3.74423895    2.25777661    8.19188400     H
    4.13934970    2.47835261    6.18089909     C
    5.99812437    4.77942748    3.09526084     H
    4.90781385    4.87103530    4.54375008     H
    3.23522800    3.30637109    5.96870678     O
    3.98784806    2.81880203    2.89980517     C
    3.66701026    1.77855909    2.67342863     H
    4.20609750    3.33043313    1.93072726     H
    3.15421594    3.34365590    3.41314271     H

outcell: Unit cell vectors (Ang):
       10.307224    0.005220   -0.190296
        5.157557    8.921327   -0.152153
       -0.490128   -0.172656   28.970497
```

Nit9 on Cu step on-top via >CO

```
    7.99958085    0.13280962   -0.10209022     Cu
    6.63406561    2.36769888   -0.06040853     Cu
    9.22594983    2.39996729   -0.08401504     Cu
    5.41393645    4.66013482   -0.15171600     Cu
    7.97513942    4.62581099   -0.02529320     Cu
   10.54191344    4.61897301   -0.12734512     Cu
    4.10095777    6.84894657   -0.13177019     Cu
    6.69590528    6.85666457   -0.14796832     Cu
    9.27354907    6.84363905   -0.18512075     Cu
   11.85139553    6.84578820   -0.16797814     Cu
    1.51775414    0.87989309   -1.97970343     Cu
    4.09442168    0.87759149   -2.01068635     Cu
    6.65451274    0.86711147   -2.18748892     Cu
    9.27041599    0.87906631   -2.17650709     Cu
    2.80291352    3.11193010   -2.01117495     Cu
    5.34913289    3.09404144   -2.19478342     Cu
    7.93406770    3.10060770   -2.19338493     Cu
   10.56566903    3.09038121   -2.17355255     Cu
    4.07318361    5.33107332   -2.22621739     Cu
    6.67596792    5.34800901   -2.26737419     Cu
    9.24904321    5.33939544   -2.27156169     Cu
   11.83623399    5.32736528   -2.24173911     Cu
    5.38870274    7.59967541   -2.23133133     Cu
```

```
    7.96513663    7.61432833   -2.23702861     Cu
   10.54092455    7.59378430   -2.27041933     Cu
   13.11941651    7.57435348   -2.28422843     Cu
    0.22661187    1.58274693   -4.30625440     Cu
    2.79473354    1.58694850   -4.18413723     Cu
    5.35925467    1.57558951   -4.33464844     Cu
    7.95082796    1.58292745   -4.38349886     Cu
    1.50936889    3.81000226   -4.34610510     Cu
    4.06802622    3.81101567   -4.35014894     Cu
    6.65688589    3.81545566   -4.40014860     Cu
    9.24045635    3.81091520   -4.37079210     Cu
    2.79374638    6.05290494   -4.42638416     Cu
    5.36757640    6.05629621   -4.42744594     Cu
    7.95220350    6.05783337   -4.43388839     Cu
   10.52908809    6.04710973   -4.45876166     Cu
    4.08223370    8.28382897   -4.43222956     Cu
    6.66216796    8.29673961   -4.38859875     Cu
    9.23918486    8.29595622   -4.41122947     Cu
   11.82133128    8.28083372   -4.45987213     Cu
    5.58885378   -1.23264786    3.92708949     H
    4.16118810   -2.00320085    3.13094615     H
    4.79268831   -1.08720689    3.16277521     C
    5.27564615   -0.95598245    2.16632791     H
    4.83012708    0.17664488    7.13981137     H
    2.43009662   -1.04477013    5.06762288     O
    3.10042238   -0.11047865    7.56760982     H
    3.82154941    0.64348293    7.18023467     C
    3.26001973   -0.08577524    4.85245671     N
    3.90261406    0.13476042    3.50177657     C
    2.13755274   -0.56227118    2.41888332     H
    3.35556249    1.10504113    5.77364408     C
    4.70347394    1.41103404    3.80370758     C
    3.85313422    1.50116428    7.88897005     H
    2.79488327    0.33798350    2.42600564     C
    5.64850096    1.98270331    2.79246710     C
    5.47571466    1.70495008    1.56684245     O
    4.38998235    1.93297314    5.02610788     C
    6.67083816    2.78708963    3.20526684     N
    6.87739522    2.94632782    4.19099591     H
    3.24014132    0.47715721    1.41734824     H
    7.27545883    3.19902216    2.47601023     H
    1.21998824    1.04194164    6.20424051     H
    4.79283560    2.87191122    5.44952199     H
    1.96392612    1.79740140    5.86404707     C
    2.16571861    1.22902368    2.64757759     H
    1.64333403    2.18211542    4.87192956     H
    1.97759391    2.64491927    6.58486469     H


outcell: Unit cell vectors (Ang):
       10.311570   -0.000428   -0.018676
        5.155071    8.928646   -0.071086
       -0.052079   -0.192451   29.687165
```

Nit9 on Cu step on-top via -NH_2

8.04464699	0.23532523	-0.31931915	Cu
6.81426512	2.45249919	-0.37438295	Cu
9.36885474	2.45605560	-0.40561900	Cu
5.50678208	4.67519543	-0.31255963	Cu
8.10126877	4.70040419	-0.39372729	Cu
10.65344038	4.69052745	-0.49740592	Cu
4.20620496	6.96689000	-0.35991141	Cu
6.79513887	6.98770480	-0.46778303	Cu
9.36279110	6.92499170	-0.51360084	Cu
11.93146726	6.91704821	-0.55051570	Cu
1.58753489	0.92507641	-1.98890028	Cu
4.18062327	0.92994521	-2.05358437	Cu
6.71624723	0.91742802	-2.41747454	Cu
9.33056077	0.91901128	-2.45674936	Cu
2.88212291	3.16724979	-2.07940025	Cu
5.40963500	3.13949607	-2.38909294	Cu
8.03199180	3.15951022	-2.53944509	Cu
10.64597421	3.13185233	-2.52438162	Cu
4.14888624	5.37680578	-2.39846822	Cu
6.72529790	5.38793120	-2.50418523	Cu
9.31701775	5.39135880	-2.62631557	Cu
11.90536344	5.37406102	-2.61965402	Cu
5.44728775	7.63562224	-2.52213341	Cu
8.03169754	7.66964267	-2.57384214	Cu
10.59975794	7.63452958	-2.64902008	Cu
13.16850392	7.61556032	-2.71368544	Cu
0.28966175	1.61469675	-4.41248306	Cu
2.84703310	1.62018032	-4.20729868	Cu
5.39425461	1.61535145	-4.51924128	Cu
7.98876704	1.61442218	-4.64830083	Cu
1.57406477	3.84107082	-4.49327296	Cu
4.11113164	3.84265049	-4.52524157	Cu
6.69045325	3.84592644	-4.64582394	Cu
9.28160479	3.84526980	-4.74109554	Cu
2.84978484	6.07898712	-4.61700237	Cu
5.41016991	6.07732909	-4.67407759	Cu
7.98314165	6.08193681	-4.74263194	Cu
10.56686138	6.07922185	-4.82595240	Cu
4.12914628	8.30528335	-4.71990620	Cu
6.70425602	8.31974312	-4.69963214	Cu
9.27604066	8.31995300	-4.76428229	Cu
11.84963673	8.30384940	-4.89728037	Cu
7.52476934	8.38978104	3.27594516	H
8.94242579	8.29027545	4.41838860	H
5.47554120	6.90434352	2.38661033	O
8.35324091	7.74812602	3.64445712	C
5.98145056	7.40963933	5.07996703	H
9.02413775	7.51883347	2.78592315	H
7.36898606	7.30487206	6.24272095	H
6.81498413	6.76881763	5.44080068	C
5.91585068	5.75072619	2.56192150	C
7.78857154	6.44523463	4.27919857	C
4.19129921	4.81941159	1.97449580	H
7.20996881	5.46596347	3.24847444	C

```
    5.20313208    4.63657553    2.03087786     N
    6.38840537    5.83787904    5.87600613     H
    9.75939170    6.06656134    5.67936303     O
   10.50750200    5.56550630    2.48043832     H
    8.93394101    5.61150767    4.80464030     N
    8.03550865    4.39259935    3.04563774     C
    5.42510262    3.71790092    2.43530767     H
   10.60201475    4.70051724    3.17453618     C
    9.26961279    4.42510202    3.93376386     C
   11.39195166    4.92989405    3.92639756     H
    7.87292107    3.58127296    2.30800201     H
   10.90708659    3.81472298    2.57257212     H
    9.39747768    3.15253652    4.81551805     C
    8.43841360    2.92330196    5.33023228     H
   10.17769323    3.32312276    5.59025299     H
    9.68787457    2.27316134    4.19807590     H

outcell: Unit cell vectors (Ang):
       10.289390   -0.001875   -0.223374
        5.143899    8.912307   -0.299553
       -0.638189   -0.606231   30.231001
```

Nit9 w/o O on Cu step on-top via NH_2

```
    8.00844064    0.14920362   -0.13787750     Cu
    6.74641103    2.39207838    0.02314943     Cu
    9.34170976    2.38234540   -0.23070010     Cu
    5.43461560    4.64909873   -0.21609575     Cu
    8.01979773    4.66412266   -0.20991306     Cu
   10.57117149    4.63889491   -0.26784742     Cu
    4.12463375    6.86588463   -0.22499583     Cu
    6.70842626    6.89672853   -0.25587199     Cu
    9.28978214    6.87948928   -0.27883239     Cu
   11.85976053    6.86033788   -0.29220784     Cu
    1.53198239    0.89199144   -1.96458576     Cu
    4.09890283    0.88470410   -2.12951244     Cu
    6.66204576    0.88181571   -2.20153884     Cu
    9.26855779    0.86969191   -2.25859450     Cu
    2.82584362    3.12171797   -2.04222556     Cu
    5.37392838    3.08067763   -2.20630659     Cu
    7.94780705    3.09537146   -2.26898853     Cu
   10.59648895    3.10210390   -2.31597732     Cu
    4.09053626    5.33391532   -2.28860030     Cu
    6.67681092    5.35793441   -2.35440775     Cu
    9.26277325    5.35986100   -2.40190236     Cu
   11.84666958    5.34300001   -2.38067985     Cu
    5.39810416    7.61387305   -2.33444525     Cu
    7.97762189    7.63219360   -2.34317982     Cu
   10.54537269    7.61539469   -2.38998563     Cu
   13.11472349    7.58561400   -2.42436024     Cu
    0.22864077    1.59102211   -4.32120251     Cu
    2.78285874    1.60033690   -4.23871826     Cu
    5.36103300    1.58819653   -4.37405153     Cu
    7.94423733    1.59275269   -4.44198244     Cu
    1.51532555    3.82712720   -4.42009872     Cu
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```
    4.07269820    3.82105164   -4.37787207     Cu
    6.65372851    3.82487232   -4.45738124     Cu
    9.23521783    3.82645087   -4.49095649     Cu
    2.80126883    6.06818590   -4.49393394     Cu
    5.36602066    6.06710351   -4.51116895     Cu
    7.94788986    6.07005797   -4.52846101     Cu
   10.52282249    6.06386601   -4.58229931     Cu
    4.08306275    8.29679768   -4.52850151     Cu
    6.65946185    8.30892789   -4.49404493     Cu
    9.23126531    8.30389928   -4.55818998     Cu
   11.81190008    8.30097015   -4.58779954     Cu
    5.67535823    4.83983908    3.29040164     H
    7.39165028    5.26393772    3.67869528     H
    6.73853948    4.56566077    3.10982472     C
    6.94715671    4.68435541    2.01973148     H
    4.17100699    3.02985502    5.94988628     H
    7.47376617    3.73709556    5.87888389     O
    5.35310015    2.85268093    7.30007485     H
    4.86968575    2.32285161    6.44835763     C
    6.79884329    3.03051332    5.04432236     N
    7.02465217    3.11489234    3.55688162     C
    9.16885632    3.39635376    3.83473937     H
    5.98266955    1.84339586    5.47541550     C
    5.99980365    2.07751250    3.05271894     C
    4.28954719    1.46133485    6.84717527     H
    8.49833909    2.71641225    3.26207517     C
    5.70501568    1.85252463    1.61453558     C
    5.47192699    1.37997263    4.11938001     C
    4.52899608    1.24738791    1.35429975     N
    3.81699234    1.05320802    2.07303256     H
    8.72682835    2.81298374    2.17185456     H
    4.27337640    1.00488762    0.37794530     H
    7.42015544    1.33797035    7.03142640     H
    4.76934006    0.52899399    4.04194728     H
    6.90583256    0.81497676    6.19368155     C
    8.70349319    1.66686293    3.56833557     H
    7.67841881    0.41368302    5.50309147     H
    6.32204910   -0.03863602    6.60398216     H

outcell: Unit cell vectors (Ang):
       10.298003   -0.000360   -0.090022
        5.148805    8.935076   -0.174373
       -0.252817   -0.417622   29.065996
```

Nit9 w/o NH_2 on Cu step on-top via CO

```
    8.08118541    0.21365953   -0.47555068     Cu
    6.78757624    2.41491393   -0.42348371     Cu
    9.43321845    2.42960671   -0.56709058     Cu
    5.50971116    4.68547531   -0.49838333     Cu
    8.11661074    4.70575740   -0.43076605     Cu
   10.68213114    4.67445647   -0.63096161     Cu
    4.21290902    6.90894228   -0.51475480     Cu
    6.78607489    6.94409195   -0.59353528     Cu
    9.36926320    6.91324260   -0.66962376     Cu
```

11.93712506	6.88951930	-0.67513806	Cu
1.57836882	0.89425301	-2.05302826	Cu
4.19242089	0.89316738	-2.16396661	Cu
6.72036914	0.90346055	-2.56168646	Cu
9.32680917	0.89614986	-2.61004029	Cu
2.88601309	3.14484773	-2.17771640	Cu
5.41264641	3.10489801	-2.51033361	Cu
8.02305310	3.13034774	-2.63108633	Cu
10.65594113	3.10212811	-2.66337937	Cu
4.14679044	5.34786408	-2.57249826	Cu
6.74558864	5.35677629	-2.64285992	Cu
9.31145723	5.35150389	-2.72279335	Cu
11.89972284	5.34433253	-2.76398386	Cu
5.45206576	7.60453003	-2.66269233	Cu
8.02079905	7.65743569	-2.71112939	Cu
10.59358514	7.60246068	-2.78831149	Cu
13.16213942	7.58769384	-2.80392090	Cu
0.29736665	1.57520503	-4.59398530	Cu
2.82481686	1.57458012	-4.27705045	Cu
5.37563918	1.57845150	-4.63710288	Cu
7.97711623	1.58681710	-4.78753935	Cu
1.57187456	3.79889388	-4.68763864	Cu
4.09529678	3.79346062	-4.65216617	Cu
6.67747179	3.80638026	-4.77698941	Cu
9.27246979	3.80976535	-4.86186487	Cu
2.84405880	6.03621133	-4.81353330	Cu
5.40259251	6.03612789	-4.80792284	Cu
7.97844655	6.04082689	-4.86255847	Cu
10.54939205	6.03427167	-4.95063334	Cu
4.12994625	8.26135991	-4.85608676	Cu
6.69295146	8.27543511	-4.83660276	Cu
9.25548665	8.28150076	-4.89173082	Cu
11.83424055	8.26744559	-4.98658624	Cu
7.81317499	2.29437618	4.64668684	H
6.67953141	1.53649025	5.85282577	H
7.79687026	3.24593068	2.08504052	O
7.00915827	1.54022525	4.78966103	C
6.04128115	4.04758429	4.06700547	H
7.42648869	0.53761488	4.54809761	H
4.86152707	3.31389156	5.23500577	H
5.23802014	3.28876738	4.18805178	C
6.98731954	2.45684890	1.55415062	C
5.79209002	1.87373219	3.88243814	C
6.07125917	1.61915761	2.39277044	C
4.39702199	3.54677737	3.50665908	H
4.15637002	0.67708609	5.26264457	O
6.15835935	-1.48801485	3.65703475	H
4.70093802	0.84974537	4.11818406	N
5.38773885	0.53008765	1.92637080	C
5.07089946	-1.52997802	3.43108684	C
4.53395088	-0.13843506	2.98491858	C
4.52931038	-1.83575532	4.35424726	H
5.44674964	0.15769926	0.88209434	H
4.90680257	-2.29273931	2.63484284	H
3.03850332	-0.23548922	2.58333498	C
2.66089344	0.72914211	2.17709378	H

```
    2.43547086   -0.51499854    3.47554546     H
    2.90595484   -1.02103567    1.79677789     H

outcell: Unit cell vectors (Ang):
       10.275357   -0.000830   -0.159764
        5.138188    8.897064   -0.183654
       -0.441082   -0.319221   29.982271
```

Nit9 w/o nitroxyl O on Cu step on-top

```
    7.90050514    0.01089977   -0.10029856     Cu
    6.59755474    2.25713237    0.22208371     Cu
    9.18897150    2.25325324   -0.09636126     Cu
    5.34190939    4.51755329   -0.01575078     Cu
    7.93006115    4.51924321   -0.03414983     Cu
   10.47710411    4.47869791   -0.15045460     Cu
    4.06871538    6.76073130   -0.05205691     Cu
    6.63409219    6.75594408   -0.11025673     Cu
    9.20637088    6.71426174   -0.17444794     Cu
   11.82115465    6.64655597   -0.15775067     Cu
    1.41176982    0.73647968   -1.96916640     Cu
    3.96843482    0.73913083   -2.05954822     Cu
    6.52496816    0.75484040   -2.09218451     Cu
    9.16565507    0.74111565   -2.18405818     Cu
    2.68518680    2.98063535   -2.01891858     Cu
    5.23241631    2.95077387   -2.03389603     Cu
    7.80255819    2.95695547   -2.11515646     Cu
   10.46074306    2.95464863   -2.20499866     Cu
    3.96545347    5.20354097   -2.10089058     Cu
    6.55230120    5.21294201   -2.18951760     Cu
    9.14278692    5.21500830   -2.25827385     Cu
   11.72780588    5.20325847   -2.27329649     Cu
    5.28793545    7.46858142   -2.17552054     Cu
    7.85917454    7.48851682   -2.21524255     Cu
   10.43690016    7.46723597   -2.25937320     Cu
   13.00953459    7.46868791   -2.22446022     Cu
    0.10564386    1.46816436   -4.27676057     Cu
    2.66896880    1.46892111   -4.20062295     Cu
    5.24343963    1.47076774   -4.24798849     Cu
    7.82578941    1.47129009   -4.33407350     Cu
    1.39274393    3.69990243   -4.33960015     Cu
    3.95655198    3.70099943   -4.25198606     Cu
    6.53234909    3.69678896   -4.30089613     Cu
    9.11062136    3.69702345   -4.33926363     Cu
    2.69187670    5.94561588   -4.33853356     Cu
    5.24675527    5.93540291   -4.35130529     Cu
    7.82764532    5.93549428   -4.38558907     Cu
   10.40554518    5.93448819   -4.46840541     Cu
    3.97199013    8.17475267   -4.31416223     Cu
    6.54525575    8.17731579   -4.33438172     Cu
    9.12206074    8.18173300   -4.37839866     Cu
   11.70927126    8.18166762   -4.37335996     Cu
    3.92150426   -0.82354329    1.95350562     H
    5.69540347   -0.63695373    2.28752033     H
    4.81946392   -0.17996917    1.77507908     C
```

```
    5.03361849   -0.17016615    0.67759714     H
    4.58565156    1.28658101    2.25530546     C
    2.40267394    1.21788396    1.78319683     H
    3.67108126    0.74144053    4.29762160     H
    4.46299576    1.30799739    3.77195457     C
    3.29746922    1.85183932    1.57753532     C
    4.76685941    0.53496270    6.40176845     H
    3.43706828    1.88749487    0.47115746     H
    5.78922521    2.13161867    1.98073372     N
    7.99421529    1.43050150    3.55558962     H
    5.04068104    1.47194573    6.69579505     N
    5.40581291    2.10119387    4.34315012     C
    3.08742492    2.88476386    1.93244906     H
    7.78293304    2.52150490    3.49891922     C
    6.26647313    2.77646722    3.25271928     C
    5.19386399    1.64323617    7.69149412     H
    5.58336318    2.39745584    5.81348474     C
    8.38419929    2.94760158    2.66076520     H
    8.10544098    3.00321310    4.44952449     H
    6.15609244    3.42353603    6.22579913     O
    5.99126389    4.31374730    3.24979313     C
    4.91672362    4.51145506    3.03315193     H
    6.60218048    4.80205146    2.45176940     H
    6.24140318    4.76323376    4.23636601     H

outcell: Unit cell vectors (Ang):
       10.302186    0.000641   -0.077922
        5.153965    8.919781    0.094291
       -0.149379    0.453866   30.319189
```

O atom on Cu hcp site

```
    0.09936520    0.05928594   -0.15699442     Cu
    2.71797561    0.06910058   -0.12951067     Cu
    5.33083323    0.08618305   -0.10882013     Cu
    7.94979526    0.09889932   -0.08266098     Cu
    1.42249611    2.32200432   -0.14552588     Cu
    4.03992432    2.33681833   -0.11631806     Cu
    6.64965483    2.34562970   -0.09615883     Cu
    9.25872708    2.35311909   -0.07631266     Cu
    2.74309782    4.58066090   -0.13020126     Cu
    5.35263582    4.58929262   -0.13246986     Cu
    7.96770260    4.60378408   -0.12079216     Cu
   10.57831055    4.61725343   -0.06324700     Cu
    4.05620139    6.83620347   -0.12456561     Cu
    6.67217737    6.84964660   -0.13026832     Cu
    9.28079113    6.85876719   -0.07226289     Cu
   11.89809091    6.86965200   -0.05161726     Cu
    1.41505820    0.80885376   -2.28000204     Cu
    4.03187305    0.82517884   -2.25808058     Cu
    6.64733215    0.82744997   -2.24400948     Cu
    9.25981766    0.84837868   -2.20926172     Cu
    2.73492832    3.07052437   -2.26676813     Cu
    5.36899097    3.08051572   -2.28233758     Cu
    7.94866792    3.09519718   -2.26591210     Cu
```

```
   10.56960053    3.10854487   -2.19857413     Cu
    4.06202045    5.33659353   -2.29234932     Cu
    6.66260482    5.34275147   -2.30112828     Cu
    9.26809971    5.36283053   -2.25717337     Cu
   11.89694776    5.36089047   -2.18800885     Cu
    5.36065236    7.57917963   -2.28719827     Cu
    7.99288699    7.58574462   -2.26643223     Cu
   10.60744813    7.61133185   -2.21478710     Cu
   13.20454928    7.62484382   -2.18372820     Cu
    0.12491136    1.54185361   -4.45369394     Cu
    2.74549790    1.55447138   -4.42574705     Cu
    5.35636471    1.55318324   -4.39869667     Cu
    7.97514757    1.56250230   -4.37881260     Cu
    1.44579618    3.80349881   -4.44321254     Cu
    4.02312369    3.80094557   -4.39293142     Cu
    6.67328039    3.75190114   -4.52084817     Cu
    9.32111345    3.82038471   -4.36396176     Cu
    2.74722059    6.06895642   -4.42443863     Cu
    5.31277863    6.10883924   -4.52759330     Cu
    8.05927976    6.12427932   -4.51216424     Cu
   10.62191303    6.10025595   -4.35708324     Cu
    4.06308229    8.33107889   -4.41748799     Cu
    6.69126326    8.36826461   -4.38307726     Cu
    9.32247380    8.35272911   -4.36793889     Cu
   11.92480653    8.35445522   -4.37177381     Cu
    6.70183950    5.33623498   -5.65067476     O

outcell: Unit cell vectors (Ang):
       10.458027    0.046741    0.100093
        5.269297    9.034133    0.038687
        0.240911   -0.037029   27.752723
```

NH_2 on Cu bridge

```
    0.10417355    0.06948918   -0.24137906     Cu
    2.75892688    0.10594680   -0.15941592     Cu
    5.40511307    0.13330550   -0.15067281     Cu
    8.05180951    0.16356474   -0.15233546     Cu
    1.45838451    2.31946370   -0.13062414     Cu
    4.10873512    2.35348663   -0.12700741     Cu
    6.75829689    2.38200902   -0.13831470     Cu
    9.39903986    2.41350413   -0.11304657     Cu
    2.81613370    4.56759691   -0.08951272     Cu
    5.44987490    4.59836020   -0.10885065     Cu
    8.09888528    4.62362180   -0.04283151     Cu
   10.75809281    4.65400983   -0.00272348     Cu
    4.15736841    6.81861347   -0.12276940     Cu
    6.80414994    6.84241404   -0.09195296     Cu
    9.45776098    6.87369158    0.00147555     Cu
   12.10894702    6.90454642    0.00817259     Cu
    1.43437843    0.80707812   -2.31486719     Cu
    4.07849196    0.83961601   -2.28112114     Cu
    6.72171231    0.86724450   -2.27265731     Cu
    9.37606678    0.90104941   -2.25278589     Cu
    2.77545592    3.04791634   -2.24839882     Cu
```

```
    5.44086987    3.08716572   -2.27696558     Cu
    8.05600507    3.12321528   -2.27556175     Cu
   10.73746130    3.13347979   -2.18490703     Cu
    4.14161237    5.30191350   -2.26508381     Cu
    6.76862495    5.32329403   -2.23050381     Cu
    9.43800150    5.34319354   -2.12705214     Cu
   12.08030111    5.38526046   -2.13762242     Cu
    5.48436979    7.52715252   -2.27919534     Cu
    8.13197036    7.58742306   -2.16214024     Cu
   10.78159224    7.60653048   -2.14154712     Cu
   13.42464734    7.63977877   -2.13928994     Cu
    0.12393396    1.49080125   -4.48081764     Cu
    2.76690207    1.52257650   -4.45028042     Cu
    5.41173024    1.56184458   -4.41087543     Cu
    8.06496874    1.58535565   -4.39843792     Cu
    1.46706409    3.73954862   -4.42208347     Cu
    4.04454741    3.75170292   -4.33663644     Cu
    6.82537659    3.81245390   -4.50066789     Cu
    9.45162262    3.83167169   -4.30997349     Cu
    2.79902253    6.00654101   -4.38249897     Cu
    5.44393489    6.06335081   -4.51106499     Cu
    8.20501128    6.09300430   -4.20672083     Cu
   10.78363275    6.08092930   -4.27060426     Cu
    4.15453637    8.25296140   -4.38226556     Cu
    6.83923660    8.28169554   -4.33561372     Cu
    9.47916716    8.31077071   -4.30444754     Cu
   12.10971470    8.33724892   -4.29653375     Cu
    6.26661463    5.00853719   -6.03097722     N
    7.01284333    5.50725271   -6.54477698     H
    5.66769205    4.54960038   -6.73752148     H

outcell: Unit cell vectors (Ang):
       10.594242    0.121492    0.110101
        5.402716    8.990016    0.135010
        0.263101    0.243887   28.496228
```

TEMPO (Au lattice vectors)

```
    5.17476327    0.82285757    5.58504013     H
    3.47483877    1.33779516    5.76284307     H
    5.06246804    2.89450936    6.97810358     H
    4.21203110    3.77734713    5.69084649     H
    6.71477401    4.27366794    5.64852101     H
    7.05350373    2.52648133    5.50932433     H
    3.03159955    2.52261822    2.19472463     H
    2.09195333    1.83607946    3.57378130     H
    2.93414601    3.41108774    3.75912151     H
    5.06959756   -0.43734893    3.56180886     H
    3.26658475   -0.31401110    3.59356242     H
    4.18925920    0.16876348    2.11225593     H
    4.64331497    4.98101342    3.76606760     H
    6.26691023    5.62054111    3.34445006     H
    5.33709779    4.67092010    2.12923899     H
    7.65191975    3.36327550    1.98117931     H
    8.29122709    4.25251575    3.42414847     H
```

```
    8.22086801    2.44636749    3.41998439     H
    5.50219074    2.25455312    3.09848658     N
    4.28211251    1.62364674    3.75569774     C
    4.44954444    1.62417209    5.30361377     C
    4.95581156    2.96579558    5.87050667     C
    6.31539962    3.31862362    5.23474031     C
    6.26494478    3.43718287    3.68366255     C
    3.01028735    2.40169564    3.29996401     C
    4.19842136    0.16797719    3.22278714     C
    5.57983384    4.75538123    3.21104041     C
    7.69752356    3.37155124    3.09073298     C
    5.54824348    2.15153307    1.80552711     O

outcell: Unit cell vectors (Ang):
        8.728290    0.119610    0.145709
        4.467464    7.928269    0.081357
        0.466402   -0.038219   24.586261
```

TEMPO (Cu lattice vectors)

```
    8.16090922    4.24209959   -7.25339335     H
    4.62799090    2.00003978   -7.32930858     H
    7.11457227    4.41080369   -9.38684247     H
    4.99312831    3.05864728   -9.42270966     H
    7.81944440    5.27134002   -7.00194022     C
    8.58540223    5.99457033   -7.36000769     H
    3.84579767    2.74916542   -7.07166583     C
    6.52035965    5.33679377   -9.19549589     C
    4.39867484    3.98491712   -9.23329377     C
    2.86496450    2.37900406   -7.44441784     H
    7.73600391    5.34665643   -5.89709556     H
    5.26567272    5.01560184  -10.95780182     H
    7.09385008    6.17625747   -9.65303026     H
    5.44707656    4.61725361   -7.02129630     N
    5.14036685    5.18018980   -9.86260202     C
    6.44659177    5.57478971   -7.65894981     C
    3.80378746    2.83797270   -5.96559182     H
    4.17254436    4.12994200   -7.70008090     C
    3.40886832    3.82609673   -9.72080601     H
    5.41459213    4.63120516   -5.72398676     O
    4.54221911    6.11625488   -9.76232899     H
    6.02311950    7.03383061   -7.31331303     C
    3.02386675    5.12999435   -7.37107330     C
    6.84443947    7.74647288   -7.55050918     H
    2.03679456    4.69729589   -7.64824645     H
    5.80113098    7.09990066   -6.22582922     H
    3.02414715    5.33848230   -6.27894212     H
    5.12028217    7.36058365   -7.87387525     H
    3.13189344    6.09604443   -7.91064223     H

outcell: Unit cell vectors (Ang):
       10.533392    0.014623    0.074101
        5.279631    9.091187    0.013978
        0.164557   -0.068882   24.508884
```

Nit8 (Au lattice vectors)

4.30028946	0.69123111	2.07851147	O
6.08245501	-0.63356261	4.81430492	H
3.09686241	-1.72080684	3.79991424	H
6.73444218	0.07878921	3.29495938	H
6.40124982	0.31683743	4.32925806	C
7.25063768	0.74056116	4.90704412	H
3.64914472	-0.51059814	5.83573742	H
2.34904811	-0.92711695	3.57881692	C
4.03858710	0.36127483	7.97548995	H
5.48288717	0.93846135	8.79492603	H
4.91932059	0.87327960	7.94560774	N
1.39586330	-1.18442583	4.09290319	H
2.17586711	-0.91406033	2.48046065	H
3.28852562	0.49977505	5.53176410	C
5.35644353	1.57056993	6.83332003	C
5.23630484	1.34108545	4.24316221	C
2.85928408	0.45764065	4.03856097	C
4.16662501	0.75401501	3.35736030	N
6.41444138	2.21970385	6.84954263	O
4.44524168	1.53552238	5.58586277	C
2.43610070	0.77316073	6.19382152	H
5.73777507	2.67718327	3.64422241	C
6.25929766	2.49012268	2.68008122	H
6.42875816	3.16711912	4.36493304	H
1.83536493	1.56390565	3.65854440	C
3.99911910	2.55912495	5.55684624	H
0.83041509	1.34619012	4.08447009	H
1.75081141	1.61048067	2.55026433	H
4.88608042	3.36411174	3.44010562	H
2.15296805	2.56793767	4.01831253	H

outcell: Unit cell vectors (Ang):

8.762238	-0.014182	0.050477
4.368670	7.556790	-0.034675
0.159601	-0.226337	27.693883

Nit8 (Cu lattice vectors)

4.19641088	0.70643794	2.01876509	O
6.01066911	-0.66683101	4.77602582	H
2.99806978	-1.77352527	3.80774228	H
6.64576235	0.01891157	3.23948281	H
6.32458321	0.27594537	4.27291868	C
7.18692736	0.70087342	4.83036298	H
3.58750461	-0.55351408	5.78308309	H
2.28881335	-0.97016016	3.50783317	C
3.95116399	0.35240417	7.93369616	H
5.41891281	0.89073062	8.73610675	H
4.85434577	0.82340340	7.88764597	N
1.28645929	-1.20577285	3.92943410	H
2.22211979	-0.96932650	2.39719349	H
3.21939856	0.45411530	5.47955599	C
5.28738703	1.52787266	6.77751726	C

```
    5.16152435    1.30374408    4.18777638     C
    2.78380378    0.41421187    3.98748324     C
    4.08675890    0.72334185    3.30200696     N
    6.34678793    2.17371380    6.78970782     O
    4.37277522    1.49553626    5.53227388     C
    2.36971581    0.72115875    6.14775941     H
    5.65951386    2.63526299    3.57927995     C
    6.10773892    2.44504224    2.57967690     H
    6.40935671    3.09828812    4.25683569     H
    1.75482867    1.51976483    3.61583435     C
    3.92552419    2.51869915    5.50821753     H
    0.73922244    1.27475377    3.99939450     H
    1.70770234    1.60714869    2.50768867     H
    4.81441835    3.34576901    3.43848384     H
    2.04823639    2.51321944    4.02293296     H

outcell: Unit cell vectors (Ang):
       10.719039    0.079345    0.046763
        5.430007    9.004870    0.110791
        0.093976    0.224175   25.589757
```

Nit9 (Au lattice vectors)

```
    4.50538679    0.99483254    3.69400482     H
    7.84166964    1.85363111    3.66535099     H
    3.82127816    1.79114059    3.32705440     C
    3.68481263    1.65825426    2.23039823     H
    8.08492648    2.91003733    3.41298573     C
    8.37709712    2.95358296    2.34047306     H
    2.83416773    1.67345576    3.82798140     H
    8.93509825    3.24515985    4.04581056     H
    5.91772819    2.75956072    7.51927584     H
    5.71369721    3.40605009    1.53298076     O
    5.70209168    3.34870703    2.81820133     N
    4.41486169    3.20114571    3.59176317     C
    6.86269846    3.83450168    3.64936016     C
    6.62186807    3.49722447    7.48329479     N
    4.93518319    3.38276309    5.00894762     C
    6.26010992    3.70641392    5.05425005     C
    7.24251319    3.60131251    8.28856299     H
    7.10592689    3.97845161    6.27234656     C
    4.26657860    3.28038136    5.88422071     H
    8.16946186    4.62212025    6.20444173     O
    3.42020546    4.31142646    3.14855094     C
    3.36017132    4.29763874    2.03687136     H
    7.19463082    5.30198143    3.25659824     C
    7.40826156    5.33603779    2.16472473     H
    2.40586406    4.13740235    3.56980974     H
    8.06988391    5.66459797    3.83582660     H
    3.76658966    5.31813016    3.47053018     H
    6.33248068    5.97381700    3.46417359     H

outcell: Unit cell vectors (Ang):
        8.875554   -0.091411   -0.038991
        4.362771    7.374388   -0.142144
       -0.034171   -0.459770   24.566997
```

Nit9 (Cu lattice vectors)

4.47946512	0.98842932	3.69385007	H
7.82025226	1.86324990	3.66935076	H
3.79439429	1.78522355	3.32922566	C
3.65752805	1.65373251	2.23255006	H
8.05912661	2.92005457	3.41501537	C
8.35090853	2.96093061	2.34241075	H
2.80783173	1.66491766	3.83005414	H
8.91036068	3.25892161	4.04417310	H
5.90547398	2.75797283	7.52146388	H
5.67540062	3.42345426	1.53306034	O
5.67185960	3.34641119	2.81720092	N
4.38596200	3.19537961	3.59562564	C
6.83165953	3.83825633	3.64903849	C
6.60294288	3.50179417	7.48246155	N
4.90863360	3.37751794	5.01195795	C
6.23183834	3.70738243	5.05433667	C
7.22834424	3.60843862	8.28370870	H
7.07992552	3.98477667	6.26959930	C
4.24341396	3.27294954	5.88947900	H
8.13880899	4.63493258	6.19641725	O
3.38862375	4.30462289	3.15510767	C
3.34307053	4.30149514	2.04270927	H
7.15101604	5.30776674	3.25603420	C
7.36500368	5.34072188	2.16437288	H
2.36952870	4.12243845	3.56175535	H
8.02148897	5.68025362	3.83565599	H
3.72746929	5.30927475	3.49068623	H
6.28247103	5.97235830	3.46037417	H

outcell: Unit cell vectors (Ang):

10.785117	0.055071	-0.033450
5.440060	9.133509	0.157827
-0.101238	0.474907	25.797129

Au 3 × 3

-0.10960360	0.07199969	-0.02539572	Au
2.81681566	0.07771357	0.01260146	Au
5.74408047	0.08456158	0.05055012	Au
1.35903743	2.60983071	-0.03764024	Au
4.28511423	2.61506520	0.00014668	Au
7.21267882	2.62283378	0.03876968	Au
2.82732582	5.14732159	-0.05040542	Au
5.75383597	5.15295636	-0.01196351	Au
8.68064617	5.15986682	0.02607286	Au
1.39401538	0.88550602	-2.51297345	Au
4.32045884	0.89139041	-2.47467068	Au
7.24786604	0.89865592	-2.43648985	Au
2.86331676	3.42351509	-2.52546542	Au
5.78947191	3.42867365	-2.48653024	Au
8.71656252	3.43573892	-2.44900420	Au
4.33122182	5.96033651	-2.53792733	Au

```
    7.25840753    5.96634525   -2.49963053     Au
   10.18480119    5.97354708   -2.46187441     Au
   -0.10667749    1.72572533   -5.00449711     Au
    2.81952817    1.73146655   -4.96616770     Au
    5.74619340    1.73765667   -4.92754150     Au
    1.36208989    4.26310834   -5.01690411     Au
    4.28890189    4.26891320   -4.97899986     Au
    7.21504827    4.27497428   -4.94019149     Au
    2.83038298    6.80055147   -5.02961110     Au
    5.75674576    6.80623980   -4.99096533     Au
    8.68318100    6.81258654   -4.95272754     Au
   -0.06752252   -0.00069369   -7.47968496     Au
    2.85834244    0.00566471   -7.44144287     Au
    5.78498416    0.01233336   -7.40247438     Au
    1.40048402    2.53700095   -7.49182098     Au
    4.32785284    2.54314259   -7.45381734     Au
    7.25394354    2.54938631   -7.41507419     Au
    2.86899355    5.07443627   -7.50418385     Au
    5.79543282    5.08073349   -7.46632594     Au
    8.72295215    5.08731890   -7.42771767     Au

outcell: Unit cell vectors (Ang):
        8.779805    0.018586    0.114529
        4.405527    7.612496   -0.037229
        0.358720   -0.354460   25.853703
```

Cu 4 × 4

```
    0.00002150    0.00016509   -0.01103229     Cu
    2.64479668    0.04874914    0.01147773     Cu
    5.28957203    0.09733257    0.03398837     Cu
    7.93434576    0.14591575    0.05649911     Cu
    1.36438288    2.26754459    0.01782430     Cu
    4.00915660    2.31612810    0.04033426     Cu
    6.65393153    2.36471095    0.06284518     Cu
    9.29870551    2.41329464    0.08535599     Cu
    2.72874263    4.53492422    0.04668134     Cu
    5.37351629    4.58350762    0.06919028     Cu
    8.01829159    4.63209132    0.09170187     Cu
   10.66306695    4.68067475    0.11421366     Cu
    4.09310325    6.80230528    0.07553840     Cu
    6.73787796    6.85088768    0.09804775     Cu
    9.38265380    6.89947244    0.12056062     Cu
   12.02742757    6.94805556    0.14307046     Cu
    1.31877952    0.75592510   -2.12170337     Cu
    3.96355436    0.80450899   -2.09919335     Cu
    6.60832781    0.85309226   -2.07668259     Cu
    9.25310229    0.90167511   -2.05417204     Cu
    2.68313990    3.02330454   -2.09284676     Cu
    5.32791323    3.07188774   -2.07033789     Cu
    7.97268565    3.12047188   -2.04782735     Cu
   10.61746281    3.16905486   -2.02531445     Cu
    4.04749884    5.29068428   -2.06399138     Cu
    6.69227266    5.33926697   -2.04148464     Cu
    9.33704756    5.38785229   -2.01897028     Cu
   11.98182347    5.43643520   -1.99645816     Cu
```

```
    5.41186101    7.55806262   -2.03513432     Cu
    8.05663609    7.60664714   -2.01262401     Cu
   10.70141036    7.65523230   -1.99011204     Cu
   13.34618403    7.70381549   -1.96760130     Cu
   -0.00284697    1.46573632   -4.25553147     Cu
    2.64193415    1.51432463   -4.23302568     Cu
    5.28670310    1.56290380   -4.21050821     Cu
    7.93147541    1.61148610   -4.18799823     Cu
    1.36151870    3.73311968   -4.22668011     Cu
    4.00629089    3.78170180   -4.20416141     Cu
    6.65106212    3.83027978   -4.18165731     Cu
    9.29583845    3.87886419   -4.15914181     Cu
    2.72587389    6.00049721   -4.19781776     Cu
    5.37064243    6.04908410   -4.17531014     Cu
    8.01542017    6.09766267   -4.15279984     Cu
   10.66019900    6.14624889   -4.13028570     Cu
    4.09023424    8.26787670   -4.16896105     Cu
    6.73501194    8.31646466   -4.14645680     Cu
    9.37978597    8.36504582   -4.12393920     Cu
   12.02455868    8.41362728   -4.10142700     Cu

outcell: Unit cell vectors (Ang):
       10.579098    0.194334    0.090043
        5.457442    9.069519    0.115427
        0.194215    0.182617   25.665578
```

Cu adatom

```
    5.61856439    3.31824459    1.93317308     Cu
    0.00492041    0.06157105    0.03601453     Cu
    2.62593702    0.09008823    0.07403394     Cu
    5.24316038    0.10786880    0.10462634     Cu
    7.86435211    0.12479621    0.10495403     Cu
    1.34011645    2.31767962    0.05419077     Cu
    3.96604753    2.35033066    0.17147660     Cu
    6.61248261    2.32107565    0.00018009     Cu
    9.19210243    2.39028091    0.13058573     Cu
    2.66099919    4.57721756    0.06078101     Cu
    5.26564830    4.65211807   -0.01885730     Cu
    7.84668811    4.59286450    0.20336276     Cu
   10.50262929    4.64526107    0.15555213     Cu
    3.98578237    6.83571768    0.03172223     Cu
    6.61270558    6.85741264    0.07228421     Cu
    9.21879603    6.87006476    0.11831666     Cu
   11.84148285    6.90299102    0.14157526     Cu
    1.33839883    0.80265933   -2.09570719     Cu
    3.95782358    0.83439517   -2.04734997     Cu
    6.57239586    0.84410847   -2.09125458     Cu
    9.18748999    0.87920302   -2.03345300     Cu
    2.67683841    3.05277080   -2.06689861     Cu
    5.27769579    3.07548004   -2.12072011     Cu
    7.90588408    3.11087798   -2.07617431     Cu
   10.52062526    3.13137285   -1.99190152     Cu
    3.98983078    5.31162347   -2.13509264     Cu
    6.62216254    5.33346925   -2.09749677     Cu
    9.22117365    5.35464545   -1.99864197     Cu
```

```
   11.84401130    5.38314640   -1.98710128     Cu
    5.32554478    7.56372447   -2.10778835     Cu
    7.94316632    7.59248912   -2.06278970     Cu
   10.55479658    7.61448199   -2.03168854     Cu
   13.17180370    7.63718872   -2.02311142     Cu
    0.02695660    1.51881365   -4.27782439     Cu
    2.64155088    1.53466582   -4.23784487     Cu
    5.25463692    1.54965338   -4.23740341     Cu
    7.87906386    1.57934039   -4.23040731     Cu
    1.35267580    3.76097596   -4.25260994     Cu
    3.96501267    3.78248820   -4.25977836     Cu
    6.59012390    3.81473289   -4.24544622     Cu
    9.20976761    3.84600529   -4.18241389     Cu
    2.67805690    6.01570425   -4.28063594     Cu
    5.29907121    6.04952940   -4.26482148     Cu
    7.92176921    6.07729048   -4.21207896     Cu
   10.53077074    6.08683261   -4.17082076     Cu
    4.00977866    8.27120349   -4.28195713     Cu
    6.63016039    8.30642064   -4.23941202     Cu
    9.24346502    8.32162776   -4.20364743     Cu
   11.86260694    8.33738023   -4.19531668     Cu

outcell: Unit cell vectors (Ang):
       10.467475    0.099633    0.121237
        5.315590    9.018389    0.014054
        0.293693   -0.146240   27.700169
```

Cu step

```
    7.85416699    0.11797971    0.06398510     Cu
    6.56566861    2.35399283    0.03835490     Cu
    9.14062940    2.35264986    0.03901610     Cu
    5.27526083    4.58677043    0.02576690     Cu
    7.85461445    4.58700033    0.10472133     Cu
   10.43214278    4.58851944    0.00916257     Cu
    3.98068134    6.82004091    0.01868383     Cu
    6.56301983    6.81791709    0.00746239     Cu
    9.14774593    6.81694196   -0.00751515     Cu
   11.73302010    6.82125479   -0.02239922     Cu
    1.40620733    0.84821056   -1.77778925     Cu
    3.98958010    0.85248452   -1.81631896     Cu
    6.54699455    0.83399282   -2.04508119     Cu
    9.16064285    0.83360607   -2.04239186     Cu
    2.69834251    3.08071773   -1.82423317     Cu
    5.23869107    3.05314895   -2.04326657     Cu
    7.85348960    3.07321373   -2.09771331     Cu
   10.46796899    3.04838634   -2.04067132     Cu
    3.96518922    5.29110614   -2.06988347     Cu
    6.56070383    5.31065569   -2.10974803     Cu
    9.14211650    5.30773966   -2.12269203     Cu
   11.73579987    5.28882114   -2.09287757     Cu
    5.27394864    7.56386685   -2.08844029     Cu
    7.85219874    7.58413622   -2.07600956     Cu
   10.42745223    7.56418456   -2.11224904     Cu
   13.00592524    7.52797657   -2.17616458     Cu
```

```
    0.10863012    1.56898988   -4.12694967     Cu
    2.67492356    1.57205095   -3.99065193     Cu
    5.24116135    1.56122907   -4.19129144     Cu
    7.83423070    1.56502587   -4.24677541     Cu
    1.39488796    3.79721963   -4.14872527     Cu
    3.94920003    3.79258819   -4.20269829     Cu
    6.53718349    3.79706620   -4.25268917     Cu
    9.12873339    3.79884407   -4.26470032     Cu
    2.67141322    6.03195907   -4.25941317     Cu
    5.24882622    6.03301036   -4.27106427     Cu
    7.83365118    6.03801198   -4.27793459     Cu
   10.41547302    6.03316366   -4.29582610     Cu
    3.95908368    8.26030720   -4.29180453     Cu
    6.54408455    8.27535740   -4.24601796     Cu
    9.12170883    8.27324457   -4.26053163     Cu
   11.69938735    8.25633507   -4.34844392     Cu

outcell: Unit cell vectors (Ang):
       10.315967   -0.003840   -0.070502
        5.153125    8.921133   -0.132160
       -0.185656   -0.304756   28.057206
```

Nit8 H-bonded dimer gas phase

```
 O    6.581578     0.961059     1.146206
 H    3.545832    -0.408750     2.092794
 H    6.015788    -2.108759     1.404295
 H    4.260544     1.102684     2.677405
 C    3.623399     0.666823     1.903011
 H    2.625137     1.106558     1.978669
 H    4.002690    -1.862902     0.126686
 C    6.567361    -1.867332     0.490309
 H    2.006316    -1.977240    -0.589181
 H    0.441193    -1.183681    -0.555014
 N    1.468822    -1.126172    -0.559361
 H    6.685212    -2.783183    -0.098590
 H    7.557677    -1.504200     0.776482
 C    4.370442    -1.187035    -0.654876
 C    2.064907     0.081743    -0.572686
 C    4.237713     0.964199     0.521373
 C    5.830228    -0.803808    -0.332523
 N    5.629486     0.423928     0.486342
 O    1.411249     1.138837    -0.557034
 C    3.590117     0.143896    -0.636741
 H    4.291555    -1.704751    -1.615970
 C    4.261377     2.473067     0.259414
 H    4.828213     2.978395     1.045649
 H    3.238587     2.855827     0.237523
 C    6.641408    -0.446146    -1.593228
 H    3.799324     0.685674    -1.567680
 H    6.845663    -1.347015    -2.181887
 H    7.594589     0.004512    -1.302795
 H    4.737964     2.694512    -0.701062
 H    6.106656     0.266838    -2.228805
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H	-6.107097	-0.267498	-2.228464
H	-6.846020	1.346404	-2.181956
C	-6.641695	0.445728	-1.593028
H	-4.738266	-2.694699	-0.700212
H	-3.799722	-0.686190	-1.567695
H	-7.594841	-0.004786	-1.302258
H	-4.291771	1.704266	-1.616626
C	-4.261450	-2.472969	0.260084
H	-3.238687	-2.855794	0.238081
C	-3.590262	-0.144125	-0.636982
C	-2.065033	-0.082070	-0.573281
C	-5.830255	0.803784	-0.332602
O	-1.411455	-1.139219	-0.557893
C	-4.370516	1.186841	-0.655366
N	-1.468844	1.125793	-0.560239
H	-4.828134	-2.978011	1.046612
C	-4.237646	-0.964018	0.521547
H	-2.006289	1.976913	-0.589425
N	-5.629399	-0.423683	0.486641
H	-0.441198	1.183233	-0.555548
O	-6.581375	-0.960548	1.146887
H	-6.685107	2.783273	-0.099173
C	-6.567184	1.867616	0.490013
H	-7.557461	1.504625	0.776501
H	-4.002600	1.862929	0.125929
C	-3.623017	-0.666229	1.902954
H	-2.624761	-1.105993	1.978537
H	-6.015424	2.109327	1.403811
H	-4.260010	-1.101810	2.677630
H	-3.545350	0.409400	2.092380

Nit9 H-bonded dimer gas phase

H	5.990616	2.067417	-1.409992
H	4.257765	-0.476209	-2.516873
C	6.487841	1.970898	-0.440573
H	7.524093	1.665095	-0.610485
C	4.201663	-1.369373	-1.886922
H	4.971297	-2.073160	-2.215828
H	6.487290	2.947834	0.054074
H	3.218610	-1.830532	-2.011631
H	1.872533	2.103447	-0.060061
O	6.862131	-1.029366	-0.504515
N	5.783874	-0.399502	-0.243598
C	5.782879	0.922310	0.440320
C	4.432509	-1.019124	-0.407170
N	1.392419	1.225749	0.057127
C	4.297955	1.152733	0.549611
C	3.562878	0.130799	0.084082
H	0.364815	1.212528	0.056282
C	2.070632	0.057337	0.062213
H	3.906638	2.063132	0.994252
O	1.492316	-1.043968	0.055680
C	6.474681	0.817759	1.814302
H	7.511322	0.498101	1.675651
C	4.337689	-2.281894	0.471464

H	5.121289	-2.982744	0.169398
H	6.470254	1.790354	2.317290
H	3.357193	-2.745108	0.351102
H	5.968427	0.091259	2.455906
H	4.479045	-2.035468	1.528084
H	-5.991403	-2.067045	-1.409837
H	-4.257948	0.476104	-2.517002
C	-6.488472	-1.970355	-0.440354
H	-7.524662	-1.664272	-0.610137
C	-4.201513	1.369260	-1.887072
H	-4.970969	2.073275	-2.215908
H	-6.488126	-2.947277	0.054322
H	-3.218342	1.830140	-2.011901
H	-1.873068	-2.104218	-0.059831
O	-6.861935	1.030013	-0.504330
N	-5.783821	0.399852	-0.243550
C	-5.783104	-0.921935	0.440411
C	-4.432299	1.019115	-0.407291
N	-1.392717	-1.226530	0.056394
C	-4.298223	-1.152772	0.549499
C	-3.562927	-0.131043	0.083873
H	-0.365130	-1.213543	0.056080
C	-2.070673	-0.057968	0.061833
H	-3.907135	-2.063304	0.994073
O	-1.492054	1.043180	0.055252
C	-6.474682	-0.817152	1.814487
H	-7.511263	-0.497236	1.675981
C	-4.337042	2.281874	0.471305
H	-5.120489	2.982923	0.169305
H	-6.470430	-1.789731	2.317507
H	-3.356437	2.744824	0.350826
H	-5.968150	-0.090759	2.455992
H	-4.478343	2.035513	1.527946

Nit9 on Cu step via CO and NH_2

7.75809742	0.03454314	0.09122556	Cu
6.32402118	2.16023486	0.08851125	Cu
9.01358133	2.26250237	0.09467925	Cu
4.98757489	4.43244697	0.07464963	Cu
7.69198245	4.49179423	0.27336841	Cu
10.32007998	4.50871846	0.18266464	Cu
3.85245461	6.73106448	0.06191681	Cu
6.40431025	6.73734239	0.07850984	Cu
9.00830688	6.75593711	0.17137013	Cu
11.58783982	6.75625995	0.19400122	Cu
1.33124873	0.79352480	-1.73029929	Cu
3.93926463	0.80086717	-1.64134864	Cu
6.46243152	0.78963492	-2.02066843	Cu
9.07501964	0.79117092	-1.98912389	Cu
2.64894153	3.04218721	-1.64483111	Cu
5.14199411	2.99424505	-2.05387037	Cu
7.73436634	3.02288883	-1.96931596	Cu
10.39083956	3.01266303	-1.89553044	Cu
3.89535489	5.23635270	-2.04478516	Cu

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     6.46339792    5.23054562   -1.97271500    Cu
     9.03447824    5.24602061   -1.90872733    Cu
    11.65318796    5.25208302   -1.88839520    Cu
     5.19193819    7.50137268   -2.01801557    Cu
     7.76774805    7.54298019   -1.91915179    Cu
    10.34223737    7.50353121   -1.90929684    Cu
    12.90622930    7.48161809   -1.99798732    Cu
     0.10300187    1.54522161   -4.13019709    Cu
     2.66645642    1.55794521   -3.83009189    Cu
     5.20405096    1.53888974   -4.18390250    Cu
     7.80022342    1.55359487   -4.18544159    Cu
     1.38574894    3.77062300   -4.05557117    Cu
     3.91923235    3.76685128   -4.19608675    Cu
     6.51097166    3.78091922   -4.19761055    Cu
     9.09033500    3.77834274   -4.09163600    Cu
     2.64756374    6.00556126   -4.21805759    Cu
     5.22810744    6.01037455   -4.20519319    Cu
     7.79766795    6.01510511   -4.10097229    Cu
    10.36797236    6.00760717   -4.07624188    Cu
     3.94277107    8.23680545   -4.22192105    Cu
     6.51900170    8.25546533   -4.10652433    Cu
     9.08507331    8.25501920   -4.03400549    Cu
    11.65322172    8.23432663   -4.17121155    Cu
     7.86117675    2.75300146    7.04919635    H
     7.12589759    3.41834605    7.55278376    C
     7.64359579    4.35879943    7.84646775    H
     6.75712626    2.91003650    8.47130921    H
     6.51764799    0.71495971    4.54775711    H
     8.15479246    3.84574614    2.83561086    H
     5.92784344    3.73122238    6.61533790    C
     6.98779279    5.05527355    5.07588116    H
     6.35585931    4.16183018    5.22684926    C
     5.20249456    2.45727536    6.27269098    N
     5.41715501    0.82104218    4.42117270    C
     4.63219317    1.73296100    7.16834221    O
     7.31608688    4.27545256    2.40184790    N
     5.83672428    3.36456586    4.21024146    C
     5.46038676    5.65617360    7.60981078    H
     4.94252328    4.71813856    7.30987973    C
     4.91908426    0.09594100    5.10389435    H
     4.94761393    2.25200428    4.79707761    C
     7.29312001    5.25557315    2.73685383    H
     4.52466214    4.23057429    8.21943806    H
     6.11481321    3.52804251    2.80403720    C
     5.15604736    0.57741905    3.36767490    H
     5.38175259    3.02573404    1.84523669    O
     4.09934013    4.98403462    6.63575372    H
     3.42920880    2.42598563    4.52296201    C
     2.87203135    1.72873523    5.18959446    H
     3.09636892    3.46292288    4.74889892    H
     3.19225710    2.20292006    3.46019169    H

outcell: Unit cell vectors (Ang):
       10.289565    0.005863    0.056542
        5.148780    8.916275    0.016267
        0.157928   -0.042810   28.517149
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