Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Application of Machine-learning-based global optimization: Potential-dependent Co-electrosorbed Structure and Activity on Pd(110) Surface

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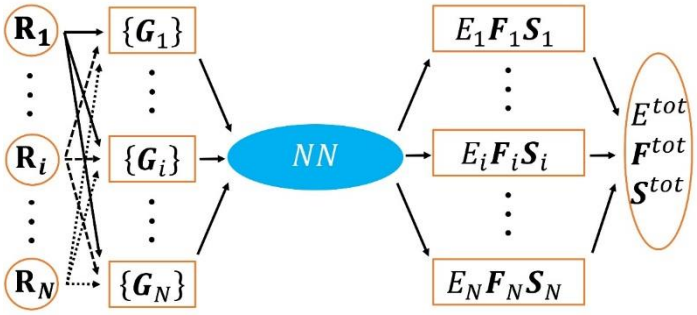
1. Theoretical Methods and Calculation detail

1.1 Architecture of neural network potential



Scheme S1. Scheme of the HDNN architecture. The subscripts (1, *i*,⋯, *N*) are atom indices and represent the total atoms in a structure. The inputs of NN are a set of structural descriptors {$\boldsymbol{G}$}, which are constructed from the Cartesian coordinates {**R**} of the structure, while the outputs of NN are the atomic properties { E_i, $\boldsymbol{F}_i$, $\boldsymbol{S}_i$ }, i.e., energies, forces, and stresses. The overall properties, E^{tot}, $\boldsymbol{F}^{tot}$, and $\boldsymbol{S}^{tot}$, can be calculated from the individual atomic contributions.

In this work, we utilized the high dimensional neural network (HDNN) scheme to construct the global NN (G-NN) potential, as shown in Scheme S1. The input nodes to NN are a set of structural descriptors of a structure, as detailedly discussed in our previous works.[1-3] The total energy E^{tot} of the structure can be composed as a linear combination of its atomic energy E^i from the output of NN

$$E^{tot} = \sum_i E_i \tag{1}$$

Consistently, the atomic force can be analytically derived from the total energy, i.e., the force component $F_{k,\alpha}$ (α = *x*, *y*, or *z*) acting on atom *k* is the derivative of the total energy E^{tot} with respect to coordinate $R_{k,\alpha}$. In combination with Eq. 1, the force component $F_{k,\alpha}$ then is related to the derivatives of the atomic energy E^i with respect to the j^{th} structural descriptors of atom *i*, $G_{j,i}$

$$F_{k,\alpha} = -\frac{\partial E^{tot}}{\partial R_{k,\alpha}} = -\sum_{i,j} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial R_{k,\alpha}} \tag{2}$$

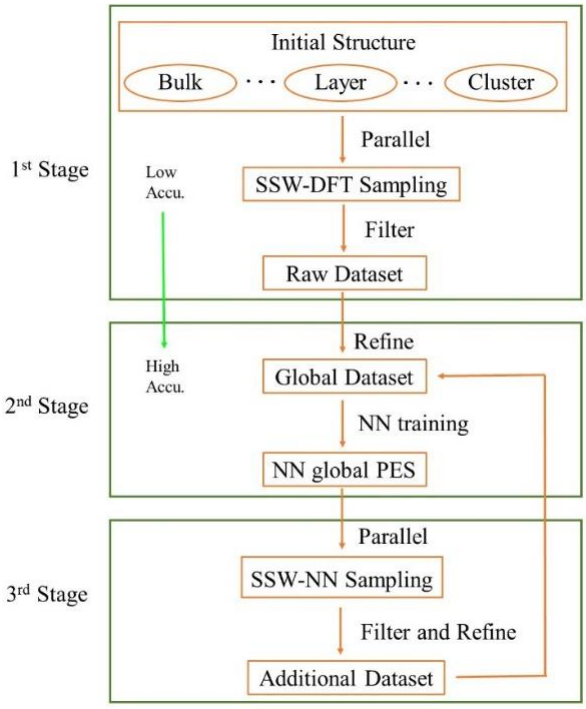
Similarly, the element $\sigma_{\alpha\beta}$ of static stress tensor matrix can be analytically derived as

$$\sigma_{\alpha\beta} = -\frac{1}{V}\sum_{i,j,d} \frac{(\boldsymbol{r}_d)_\alpha (\boldsymbol{r}_d)_\beta}{r_d} \frac{\partial E_i}{\partial G_{j,i}} \frac{\partial G_{j,i}}{\partial r_d} \tag{3}$$

where $\boldsymbol{r}_d$ and r_d are the distance vector, constituted by $G_{j,i}$ and its module, respectively, and *V* is the volume of the structure.

1.2 Generation of global dataset using SSW-NN

The quality of the potential energy surface (PES) of G-NN is largely determined by its training dataset. Here we utilized the stochastic surface walking (SSW) global optimzation[4-6] to generate a global dataset, which is fully automated and does not need a priori knowledge on the system, such as the structural motif, e.g. bonding patterns and symmetry. In brief, the SSW-NN method involves three stages to generate the global dataset, as described below.



Scheme S2. Procedure for the generation of the global training dataset by SSW global optimization. In the first stage, the SSW sampling is typically performed by low accuracy DFT calculations. In the second stage, the global dataset is first refined with high accuracy DFT setups, and then a NN training is performed based on the accurate global dataset. In the third stage, an additional dataset is generated by SSW sampling utilizing the previously obtained NN PES, and is fed into the global dataset. A new cycle of NN training then starts based on the new global dataset (back to stage 2).

In brief, the SSW-NN method involves three stages to generate the global dataset (see Scheme S2), as described below.

(i) The first stage generates a raw dataset, which contains the most common atomic environment and serves to build an initial NN PES. This is done by performing density functional theory (DFT) SSW global optimization in a massively parallel way. In this stage, the DFT calculations have low accuracy setups and small unit cells to speed up the SSW search. By collecting and screening the structures from SSW trajectories, a raw dataset is obtained.

(ii) The second stage trains a NN global PES. This is done by refining the dataset using DFT calculations with high accuracy setups, followed by NN training on the accurate global dataset (see our previous work[7] for details). The NN architecture applied in this stage utilizes a small set of structural descriptors and a small network size.

(iii) The third stage iteratively expands the global dataset. It targets to increase the predictive power of NN PES by incorporating more structural patterns into the dataset. This is done by performing SSW PES search using the NN PES obtained in the second stage, starting from a variety of initial structures. These initial structures are randomly constructed, and also include large systems with many atoms per unit cell. The structures from all the SSW trajectories are collected and filtered to generate an additional dataset. The new dataset is then fed to the global dataset to start a new cycle of NN training (back to stage 2). For example, our final dataset for training the G-NN of Pd-H system contains 18738 structures. To pursue a high accuracy for PES, we have adopted a large set of power-type structure descriptors (PTSDs), which contains 166 descriptors for every element with only power-type structure descriptors, including 95 two-body, 63 three-body, 8 four-body descriptors, and compatibly, the network utilized is also large involving three-hidden layers. Min-max scaling is utilized to normalization the training data sets. Hyperbolic tangent activation functions were used for the hidden layers, while a linear transformation was applied to the output layer of all networks. The limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) method is used to minimize the loss function to match DFT energy, force and stress. The final energy and force criterions of the root mean square errors are around 2.808 meV/atom and 0.060 eV/ Å respectively.

1.3 Benchmark of G-NN potential against DFT calculations

To examine the accuracy of the G-NN potential, we have calculated the total energy difference between G-NN and DFT for the representative surface structures of H_nPd, which shows the mean error between DFT energy and NN energy is 3.52 meV/atom**.** It is quite standard for NN potentials and accurate enough for searching the stable structure candidates. The details for the comparison between DFT and NN results can be found in **Table S1**.

Table S1. Benchmark of NN calculations for H_{r_i}Pd systems as compared with DFT results. Listed data include the compositions, total atom number (N_{atom}), DFT energy, NN energy and energy differences between DFT energy and NN energy (E_{diff}, meV/atom).

composition	N_{atom}	DFT-en (eV)	NN-en (eV)	E_{diff} (meV/atom)
H15Pd66	81	-386.0789	-386.4090	4.08
H16Pd66	82	-389.9915	-390.3317	4.15
H18Pd66	84	-397.8536	-398.1436	3.45
H19Pd66	85	-401.6662	-401.9627	3.49

H20Pd66	86	-405.4500	-405.7728	3.75
H21Pd66	87	-409.1982	-409.5663	4.23
H22Pd66	88	-412.8209	-413.0377	2.46
H23Pd66	89	-416.3344	-416.6107	3.10
H24Pd66	90	-419.9015	-420.1659	2.94

*Mean error between DFT energy and NN energy is 3.52 meV/atom.

1.4 Stochastic surface walking (SSW) global Structure Search

The potential energy surface (PES) of electrosorbed H_{r_i}-NH_y/Pd(110) phase was explored using SSW-NN global structure search. The SSW method is capable of surmounting the high barrier on PES and identifying low energy minima. The efficiency of the method for exploring PES has been demonstrated for both aperiodic (molecules,[8] clusters[9-11]) and periodic (surfaces,[12] crystals[8, 13]) systems. The algorithm of the SSW global optimization method can be found in our previous.[14-16] The key SSW parameters utilized are the same with those utilized previously for exploring PES of carbon and boron,[11, 15] i.e. the Gaussian with being 0.6 Å, the number of Gaussian bias potential being 10.

The H_{r_i}-NH_y/Pd(110) structure at different compositions has been investigated in the Pd(110) supercell periodic calculations by recently developed SSW-NN method. It is reasonable to focus on the adsorbed structures at top two layers of Pd(110) with different H_{r_i}/Pd ratios, where the bottom surface is block by the fully covered hydrogen. The NN simulation is at least 3~4 orders of magnitude faster than DFT, while keeping the accuracy in energy and force comparable with those from DFT. The combination of SSW with NN potential thus allows to fast obtain the global PES of more complex materials.[15, 16] The SSW-NN method to explore PES can be divided into three steps: (i) global dataset generation based on DFT calculations using selected structures from SSW simulation, (ii) G-NN potential fitting and (iii) SSW global optimization using G-NN potential. These steps are iteratively performed until the NN potential is transferable and robust enough to describe the global PES and more details can be found in our previous work.[17] The global minima at the key composition of H_{θ_i}Pt as identified from the SSW-NN simulation, where each composition is simulated in the unit cells of ~200 atoms and explored to cover more than 10^7 structures on PES by SSW. Thus, a large variety of structures have been obtained from SSW-NN simulation. All the low energy structure candidates from SSW-NN exploration are finally verified by DFT calculations with high accuracy setups.

1.5 DFT calculation on H_{r_i}-NH_y/Pd(110) system

All DFT calculations were performed using the SIESTA package with numerical atomic orbital basis sets[18, 19] and Troullier-Martins normconserving pesudopotentials.[20] The exchange-correlation functional utilized was at the generalized gradient approximation level, known as GGA-PBE.[21] The

optimized double-ζ plus (DZP) polarization basis set was employed. For the Pd(110) surfaces, we utilized $p(3\times2)$ (12 atoms per layer) six-layer slabs with top two layers being relaxed at the bulk-truncated position, where the bottom surface have been occupied by adsorbed hydrogen fully and fixed. The solid-liquid interface was described using the periodic continuum solvation model based on the modified Poisson-Boltzmann equation (CM-MPB), which can take into account the solvation and potential effect.[22-24] The charged-slab DFT/CM-MPB method developed previously[22, 24, 25] are utilized to add explicit charge onto the surface and the neutralizing countercharge are added into solvation following the MPB equation. The addition of surface excess charge will shift the electrochemical potential of system (the potential difference between Fermi level and the potential in solution) and thus can be determined explicitly via DFT/CM-MPB method. It should be mentioned that DFT calculations have been utilized to validate the low energy structures and confirm the identified global minimum. All energetics reported in this work are from DFT without specifically mentioning. The accuracy of the calculated energetics was examined by benchmarking the results from SIESTA with those from the plane-wave methodology and the difference in adsorption energy is generally below 0.06 eV for H (e.g, the H free energy of adsorption (with respect to the free energy of the gas-phase H_2 at the standard state) at $H_{0.5}Pd$ is calculated to be -0.24 eV from SIESTA, and it is -0.29 eV from the plane-wave method).

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2. The optimized structures of H_{r_i}/Pd(110) and H_{r_i}-NH_y/Pd(110) phases

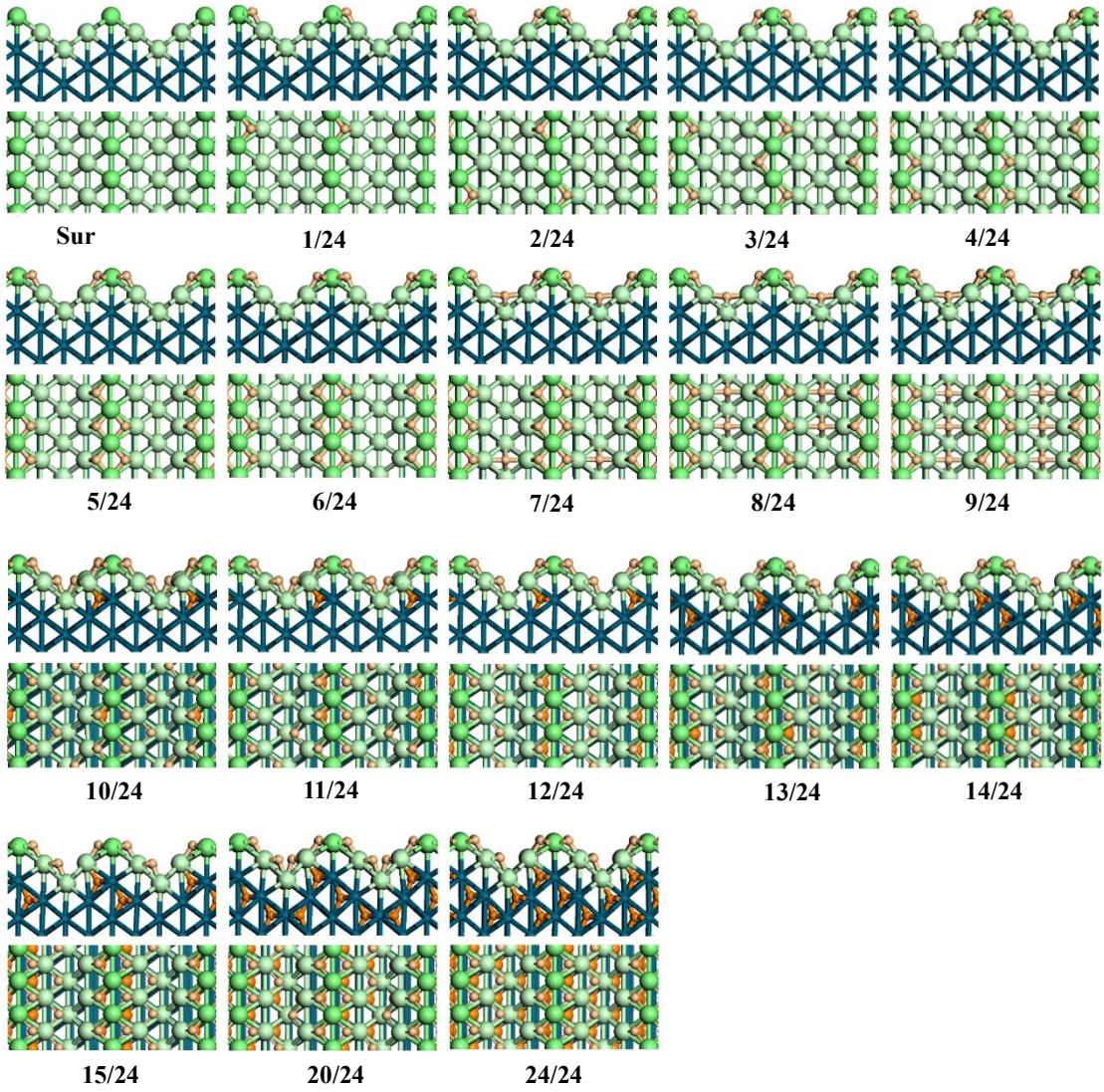


Figure S1. The optimized stable structures of different H_{r_i}/Pd(110) ratios. Large green ball: surface ridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

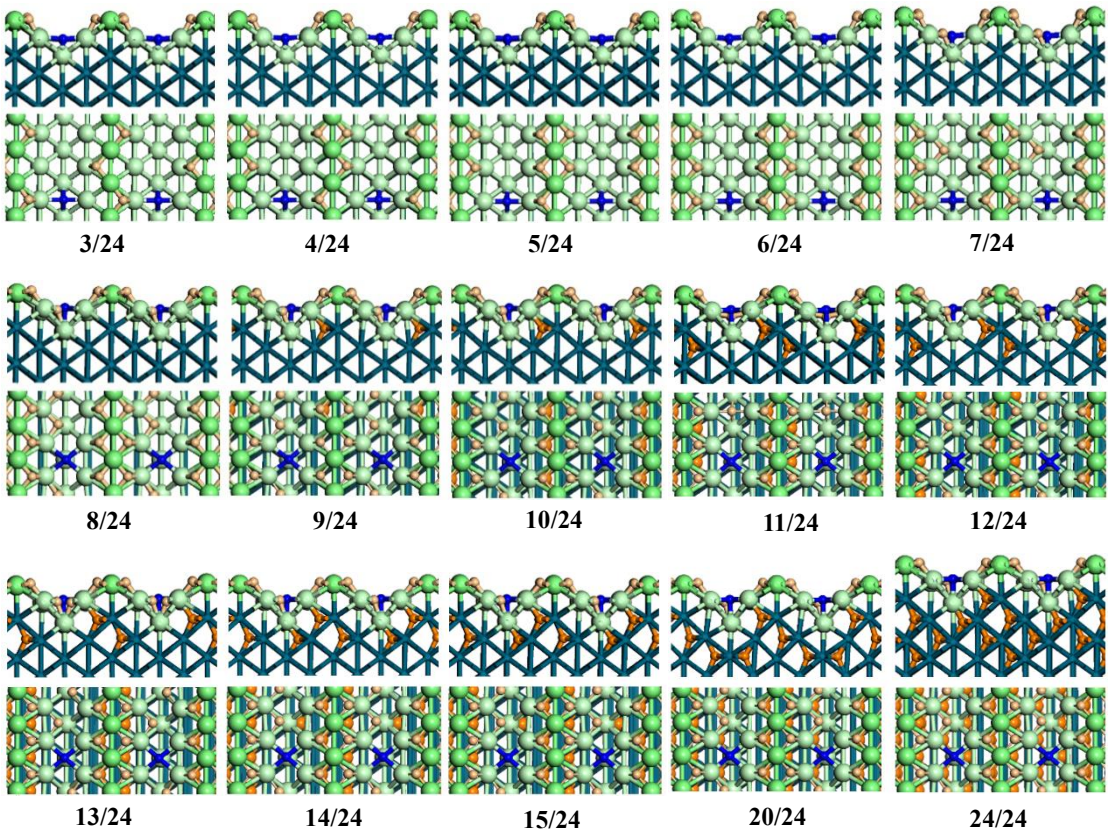
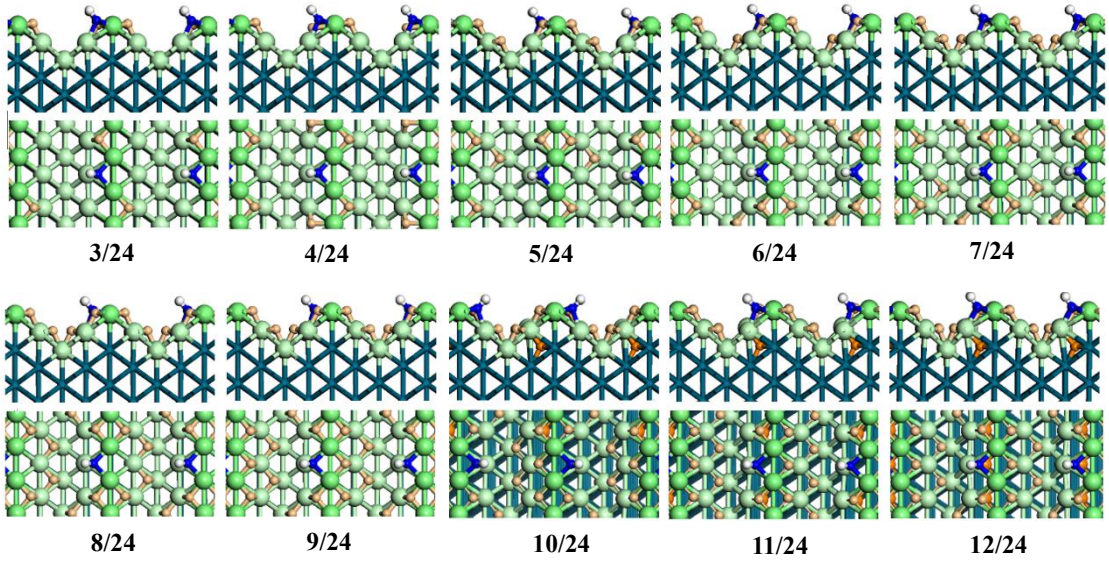


Figure S2. The optimized stable structure of the co-electrosorbed H_{r_i}-N/Pd(110) surface phases at different $H_{r_i}/Pd(110)$ ratios. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.



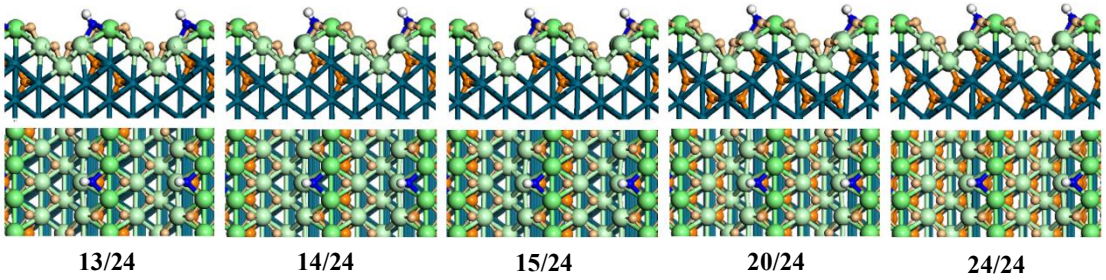


Figure S3. The optimized stable structure of the co-electrosorbed H_{r_i}-NH/Pd(110) surface phases at different $H_{r_i}/Pd(110)$ ratios. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

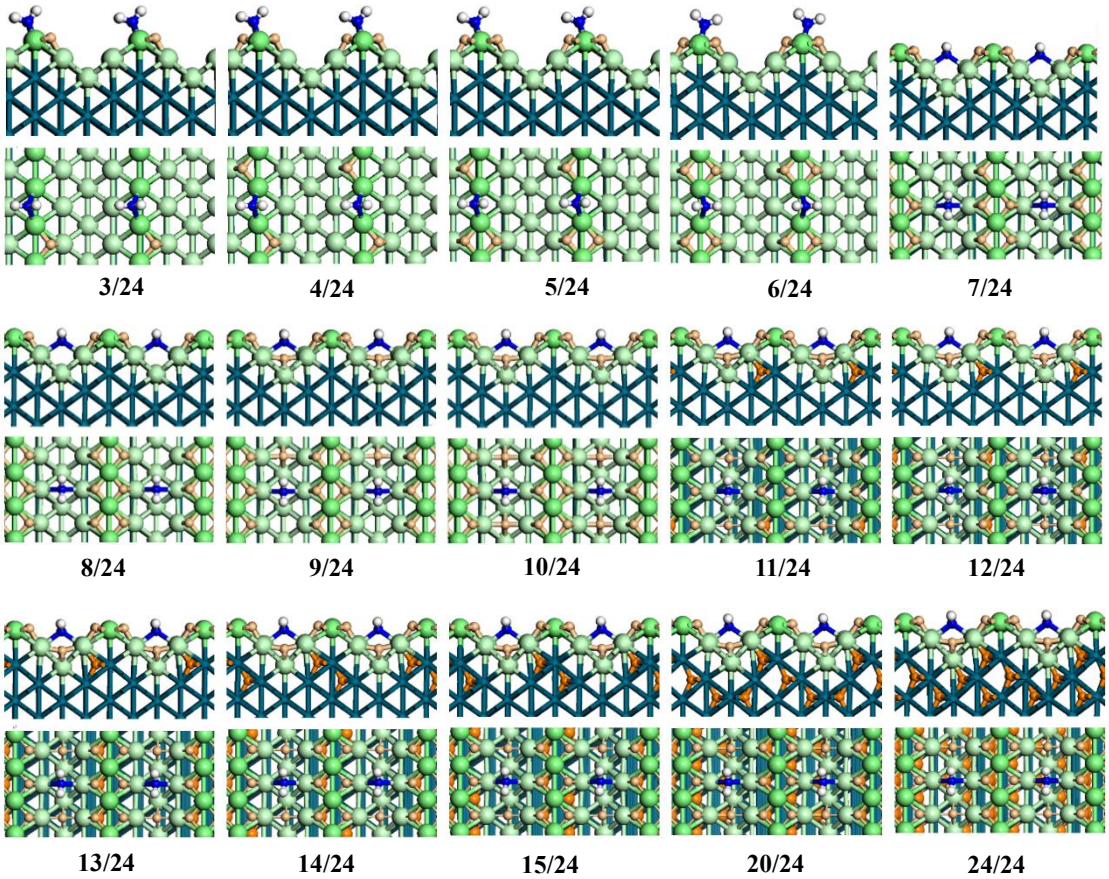


Figure S4. The optimized stable structure of the co-electrosorbed H_{r_i}-NH_2/Pd(110) surface phases at different $H_{r_i}/Pd(110)$ ratios. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

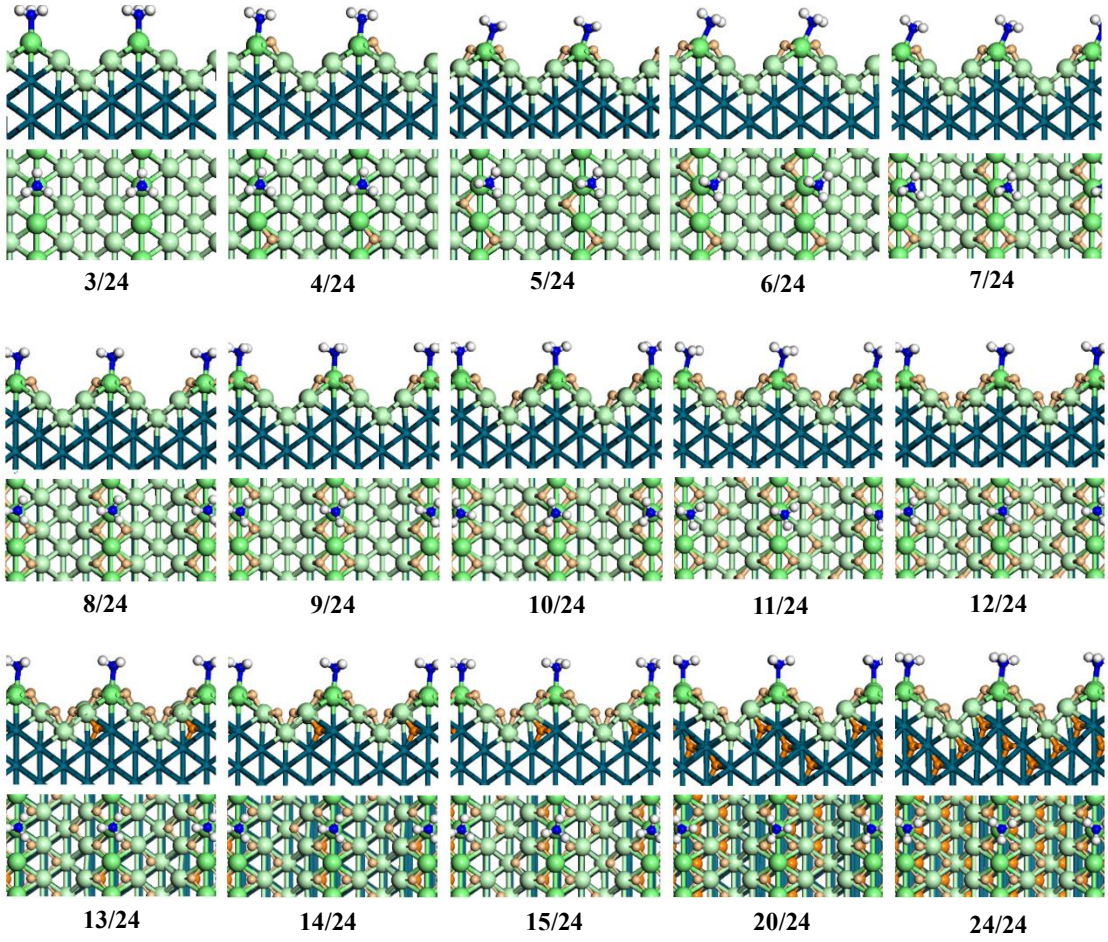


Figure S5. The optimized stable structure of the co-electrosorbed H_{r_i}-NH_3/Pd(110) surface phases at different $H_{r_i}/Pd(110)$ ratios. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

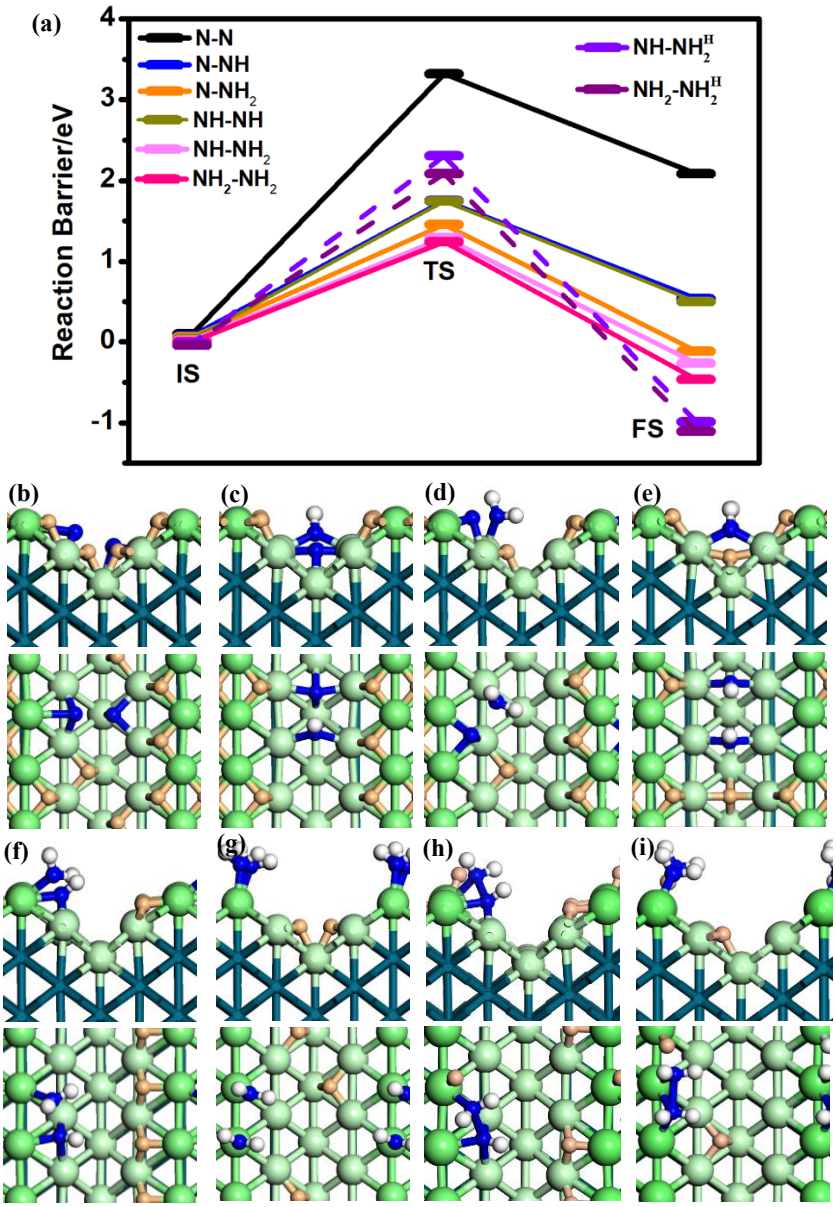


Figure S6. (a)The reaction barriers of H_yN-NH_y (N-N, N-NH, N-NH_2, NH-NH, NH-NH_2 and NH_2-NH_2) directly dissociation and H-associative H_yN-NH_y dissociation ($NH\text{-}NH_2^H$ (NH-NH_2+H→NH_3+ NH) and $NH_2\text{-}NH_2^H$ (NH_2-NH_2+H→NH_3+NH_2)) at 0.25 V. The optimized structures of transition states for (b) N-N, (c) N-NH, (d) N-NH_2, (e) NH-NH, (f) NH-NH_2, (g) NH_2-NH_2, (h) $NH\text{-}NH_2^H$ and (i) $NH_2\text{-}NH_2^H$. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small pale orange ball: surface H atoms

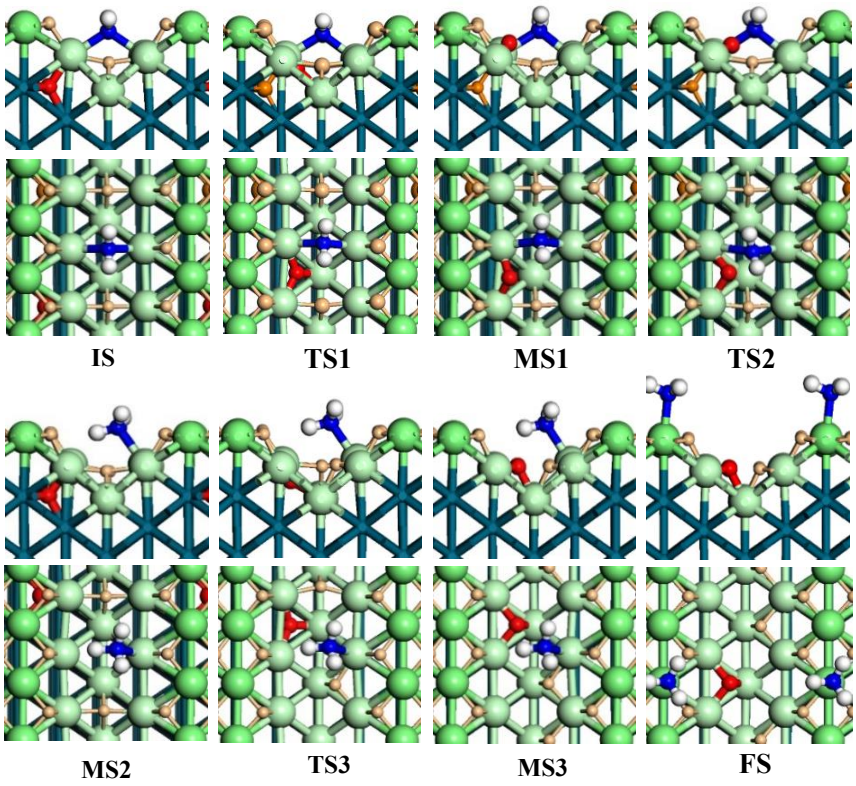


Figure S7. The optimized structures of intermediate states for NH_2 and H coupling at 0.5 ratio hydrogen. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small red ball: reactive H atom, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

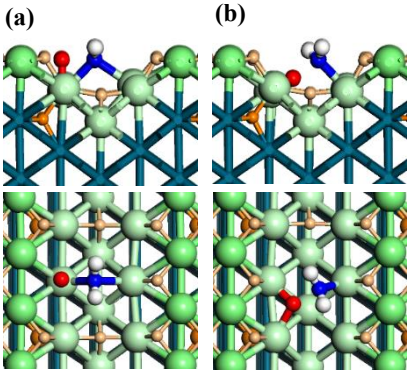


Figure S8. The optimized transition state (TS) structures of NH_2 coupling with (a) surface fcc and (b) valley bridge H atoms at 0.5 ratio. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small red ball: reactive H atom, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

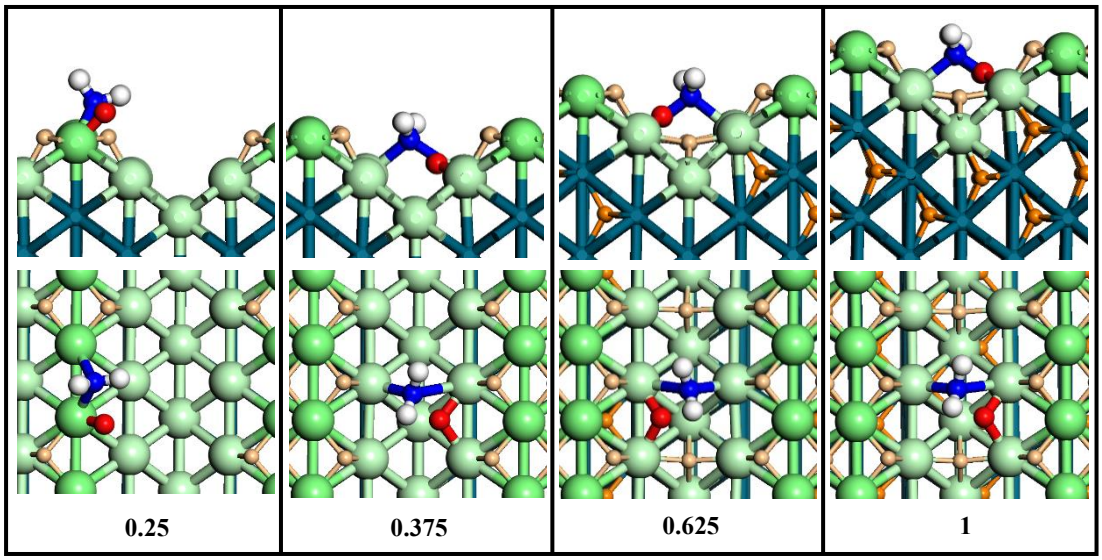


Figure S9. The optimized TS structures for NH_2 and H coupling at 0.25、0.375、0.625 and 1 hydrogen ratio. Large green ball: surface bridge Pd atoms, Large pale green ball: surface terrace Pd atoms, Blue ball: N atoms, Small red ball: reaction H atom, Small pale orange ball: surface H atoms, Small orange ball: subsurface H atoms.

3. XYZ coordinates for the structures in Fig. 1

H_{r_i}/Pd(110) ($r_i = 0$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
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Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
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Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.937436000	0.000515000	24.775895000	XXXX	1	xx	Pd 0.000
Pd56	3.937412000	2.784530000	24.775805000	XXXX	1	xx	Pd 0.000
Pd57	3.937432000	5.568543000	24.776028000	XXXX	1	xx	Pd 0.000
Pd58	2.016582000	1.394042000	29.039665000	XXXX	1	xx	Pd 0.000
Pd59	2.016435000	4.177533000	29.039795000	XXXX	1	xx	Pd 0.000
Pd60	2.016459000	6.962066000	29.039805000	XXXX	1	xx	Pd 0.000
Pd61	0.001097000	0.000361000	30.350024000	XXXX	1	xx	Pd 0.000
Pd62	0.001077000	2.784416000	30.350055000	XXXX	1	xx	Pd 0.000
Pd63	0.001086000	5.568389000	30.350003000	XXXX	1	xx	Pd 0.000
Pd64	5.861679000	1.393696000	29.042750000	XXXX	1	xx	Pd 0.000

Pd65	5.861717000	4.177735000	29.042743000	XXXX	1	xx	Pd 0.000
Pd66	5.861615000	6.961695000	29.042556000	XXXX	1	xx	Pd 0.000
Pd67	0.003386000	0.005744000	27.590458000	XXXX	1	xx	Pd 0.000
Pd68	0.003306000	2.789735000	27.590600000	XXXX	1	xx	Pd 0.000
Pd69	0.003537000	5.573760000	27.590314000	XXXX	1	xx	Pd 0.000
Pd70	1.978305000	1.393986000	26.193544000	XXXX	1	xx	Pd 0.000
Pd71	1.978205000	4.177801000	26.193402000	XXXX	1	xx	Pd 0.000
Pd72	1.978320000	6.961813000	26.193435000	XXXX	1	xx	Pd 0.000
Pd73	3.940755000	0.003058000	27.645799000	XXXX	1	xx	Pd 0.000
Pd74	3.940584000	2.786848000	27.645488000	XXXX	1	xx	Pd 0.000
Pd75	3.941833000	5.571712000	27.646016000	XXXX	1	xx	Pd 0.000
Pd76	5.897798000	1.393736000	26.189901000	XXXX	1	xx	Pd 0.000
Pd77	5.897719000	4.178005000	26.189905000	XXXX	1	xx	Pd 0.000
Pd78	5.897525000	6.961850000	26.190086000	XXXX	1	xx	Pd 0.000
end							

H_{r_i}/Pd(110) ($r_i = 0.25$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	-0.000251000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	-0.000501000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000

H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.937876000	8.351777000	24.772164000	XXXX	1	xx	Pd 0.000
Pd56	3.937854000	2.784537000	24.769067000	XXXX	1	xx	Pd 0.000
Pd57	3.937876000	5.567334000	24.769181000	XXXX	1	xx	Pd 0.000
Pd58	2.075540000	1.394306000	29.031075000	XXXX	1	xx	Pd 0.000
Pd59	2.078730000	4.176487000	29.031239000	XXXX	1	xx	Pd 0.000
Pd60	2.077221000	6.959638000	29.029828000	XXXX	1	xx	Pd 0.000
Pd61	-0.000199000	8.351676000	30.433067000	XXXX	1	xx	Pd 0.000
Pd62	-0.000433000	2.787880000	30.432241000	XXXX	1	xx	Pd 0.000
Pd63	-0.000457000	5.566584000	30.432319000	XXXX	1	xx	Pd 0.000
Pd64	5.801097000	1.394162000	29.028706000	XXXX	1	xx	Pd 0.000
Pd65	5.798156000	4.176631000	29.029125000	XXXX	1	xx	Pd 0.000
Pd66	5.799506000	6.959943000	29.027638000	XXXX	1	xx	Pd 0.000
Pd67	0.001093000	8.352045000	27.613339000	XXXX	1	xx	Pd 0.000
Pd68	0.001142000	2.785395000	27.610803000	XXXX	1	xx	Pd 0.000
Pd69	0.001167000	5.566826000	27.610845000	XXXX	1	xx	Pd 0.000
Pd70	1.954560000	1.389838000	26.177030000	XXXX	1	xx	Pd 0.000
Pd71	1.953550000	4.176255000	26.175335000	XXXX	1	xx	Pd 0.000
Pd72	1.956188000	6.963315000	26.178126000	XXXX	1	xx	Pd 0.000
Pd73	3.935867000	8.354778000	27.595309000	XXXX	1	xx	Pd 0.000
Pd74	3.935998000	2.787672000	27.584523000	XXXX	1	xx	Pd 0.000
Pd75	3.936086000	5.569383000	27.584325000	XXXX	1	xx	Pd 0.000
Pd76	5.918197000	1.389248000	26.177350000	XXXX	1	xx	Pd 0.000
Pd77	5.919545000	4.176032000	26.175381000	XXXX	1	xx	Pd 0.000
Pd78	5.916735000	6.963313000	26.178443000	XXXX	1	xx	Pd 0.000
H79	1.197545000	1.393073000	30.581709000	XXXX	1	xx	H 0.000
H80	1.197004000	4.176652000	30.582539000	XXXX	1	xx	H 0.000
H81	1.197464000	6.960325000	30.581431000	XXXX	1	xx	H 0.000
H82	6.672669000	1.393060000	30.583812000	XXXX	1	xx	H 0.000
H83	6.673315000	4.176699000	30.584712000	XXXX	1	xx	H 0.000
H84	6.672762000	6.960454000	30.583555000	XXXX	1	xx	H 0.000

end

H_{r_i}/Pd(110) ($r_i = 0.375$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000

Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.935631000	8.353426000	24.786501000	XXXX 1	xx	Pd	0.000
Pd56	3.935845000	2.786337000	24.787100000	XXXX 1	xx	Pd	0.000
Pd57	3.935830000	5.568245000	24.786607000	XXXX 1	xx	Pd	0.000
Pd58	1.872731000	4.177747000	29.125158000	XXXX 1	xx	Pd	0.000
Pd59	5.994154000	1.392897000	29.123145000	XXXX 1	xx	Pd	0.000
Pd60	3.935962000	2.785770000	30.544774000	XXXX 1	xx	Pd	0.000
Pd61	5.994513000	6.962984000	29.121433000	XXXX 1	xx	Pd	0.000
Pd62	1.871949000	6.961925000	29.127817000	XXXX 1	xx	Pd	0.000
Pd63	3.926917000	8.346903000	30.552540000	XXXX 1	xx	Pd	0.000
Pd64	3.936091000	5.567719000	30.544909000	XXXX 1	xx	Pd	0.000
Pd65	1.871669000	1.394589000	29.129591000	XXXX 1	xx	Pd	0.000
Pd66	5.996308000	4.177267000	29.120293000	XXXX 1	xx	Pd	0.000
Pd67	7.872600000	5.571608000	27.586017000	XXXX 1	xx	Pd	0.000
Pd68	7.873037000	8.360224000	27.594414000	XXXX 1	xx	Pd	0.000
Pd69	7.872864000	2.788957000	27.586512000	XXXX 1	xx	Pd	0.000
Pd70	1.987819000	1.393133000	26.201810000	XXXX 1	xx	Pd	0.000
Pd71	1.987862000	4.179045000	26.201349000	XXXX 1	xx	Pd	0.000
Pd72	1.987309000	6.965219000	26.202075000	XXXX 1	xx	Pd	0.000
Pd73	3.934257000	5.571540000	27.679426000	XXXX 1	xx	Pd	0.000
Pd74	3.930906000	0.006604000	27.685151000	XXXX 1	xx	Pd	0.000
Pd75	3.934219000	2.788992000	27.679905000	XXXX 1	xx	Pd	0.000
Pd76	5.882173000	6.965629000	26.201771000	XXXX 1	xx	Pd	0.000
Pd77	5.881739000	1.392442000	26.201407000	XXXX 1	xx	Pd	0.000
Pd78	5.882235000	4.178861000	26.200068000	XXXX 1	xx	Pd	0.000
H79	5.135716000	4.174834000	30.697954000	XXXX 1	xx	H	0.000
H80	-0.003643000	6.960673000	28.896063000	XXXX 1	xx	H	0.000
H81	2.743167000	4.174648000	30.701533000	XXXX 1	xx	H	0.000
H82	-0.003704000	1.394504000	28.897958000	XXXX 1	xx	H	0.000
H83	5.130341000	1.389416000	30.701778000	XXXX 1	xx	H	0.000
H84	2.739228000	6.954253000	30.705180000	XXXX 1	xx	H	0.000
H85	2.739802000	1.393732000	30.706733000	XXXX 1	xx	H	0.000
H86	5.131108000	6.959327000	30.700048000	XXXX 1	xx	H	0.000
H87	-0.002173000	4.177744000	28.896321000	XXXX 1	xx	H	0.000

end

H_{r_i}/Pd(110) ($r_i = 0.5$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000

Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.954560000	8.349423000	24.789523000	XXXX	1	xx	Pd 0.000
Pd56	3.954317000	2.781400000	24.789535000	XXXX	1	xx	Pd 0.000
Pd57	3.954535000	5.565443000	24.789588000	XXXX	1	xx	Pd 0.000
Pd58	1.750997000	4.164671000	29.239422000	XXXX	1	xx	Pd 0.000
Pd59	1.751068000	6.948732000	29.239527000	XXXX	1	xx	Pd 0.000
Pd60	1.750888000	1.380788000	29.239255000	XXXX	1	xx	Pd 0.000
Pd61	6.041667000	4.164470000	29.202234000	XXXX	1	xx	Pd 0.000
Pd62	6.041659000	6.948280000	29.202245000	XXXX	1	xx	Pd 0.000
Pd63	6.041917000	1.379990000	29.201906000	XXXX	1	xx	Pd 0.000
Pd64	3.916196000	8.337996000	30.556516000	XXXX	1	xx	Pd 0.000
Pd65	3.916131000	2.770920000	30.556546000	XXXX	1	xx	Pd 0.000
Pd66	3.916245000	5.554895000	30.556543000	XXXX	1	xx	Pd 0.000
Pd67	0.016351000	5.559254000	27.592486000	XXXX	1	xx	Pd 0.000
Pd68	0.016193000	8.343452000	27.592648000	XXXX	1	xx	Pd 0.000
Pd69	0.016402000	2.775072000	27.592533000	XXXX	1	xx	Pd 0.000
Pd70	1.966541000	1.383617000	26.170244000	XXXX	1	xx	Pd 0.000
Pd71	1.966516000	4.167716000	26.170211000	XXXX	1	xx	Pd 0.000
Pd72	1.966540000	6.951429000	26.170177000	XXXX	1	xx	Pd 0.000
Pd73	4.024138000	8.343384000	27.705538000	XXXX	1	xx	Pd 0.000
Pd74	4.024085000	2.775274000	27.705530000	XXXX	1	xx	Pd 0.000
Pd75	4.024144000	5.559267000	27.705561000	XXXX	1	xx	Pd 0.000
Pd76	5.922707000	1.386094000	26.196117000	XXXX	1	xx	Pd 0.000
Pd77	5.922657000	4.170193000	26.196058000	XXXX	1	xx	Pd 0.000
Pd78	5.922670000	6.954139000	26.196083000	XXXX	1	xx	Pd 0.000

H79	7.233313000	2.771363000	29.266114000	XXXX	1	xx	H 0.000
H80	2.738432000	4.161935000	30.745820000	XXXX	1	xx	H 0.000
H81	5.086864000	6.945794000	30.739584000	XXXX	1	xx	H 0.000
H82	2.807386000	4.165366000	27.781998000	XXXX	1	xx	H 0.000
H83	2.807380000	6.949359000	27.781994000	XXXX	1	xx	H 0.000
H84	2.738424000	1.377976000	30.745857000	XXXX	1	xx	H 0.000
H85	7.233296000	5.555363000	29.266117000	XXXX	1	xx	H 0.000
H86	2.738490000	6.946000000	30.745767000	XXXX	1	xx	H 0.000
H87	5.086919000	4.161794000	30.739619000	XXXX	1	xx	H 0.000
H88	5.086995000	1.377819000	30.739704000	XXXX	1	xx	H 0.000
H89	7.233194000	8.339444000	29.266008000	XXXX	1	xx	H 0.000
H90	2.807399000	1.381370000	27.781960000	XXXX	1	xx	H 0.000

end

H_{r_i}/Pd(110) ($r_i = 0.625$)

Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000

Pd55	3.924928000	0.000773000	24.760223000	XXXX 1	xx	Pd	0.000
Pd56	3.924736000	2.785184000	24.760131000	XXXX 1	xx	Pd	0.000
Pd57	3.924745000	5.569204000	24.759843000	XXXX 1	xx	Pd	0.000
Pd58	1.760438000	6.965317000	29.383990000	XXXX 1	xx	Pd	0.000
Pd59	1.760294000	1.397451000	29.384561000	XXXX 1	xx	Pd	0.000
Pd60	1.761655000	4.181803000	29.381818000	XXXX 1	xx	Pd	0.000
Pd61	6.064872000	4.182404000	29.286174000	XXXX 1	xx	Pd	0.000
Pd62	6.065291000	6.966079000	29.287201000	XXXX 1	xx	Pd	0.000
Pd63	6.066997000	1.397922000	29.288667000	XXXX 1	xx	Pd	0.000
Pd64	3.952197000	0.007837000	30.698119000	XXXX 1	xx	Pd	0.000
Pd65	3.951834000	2.791362000	30.697141000	XXXX 1	xx	Pd	0.000
Pd66	3.951690000	5.575564000	30.696847000	XXXX 1	xx	Pd	0.000
Pd67	0.076065000	5.572132000	27.689466000	XXXX 1	xx	Pd	0.000
Pd68	0.074092000	0.004539000	27.691831000	XXXX 1	xx	Pd	0.000
Pd69	0.075250000	2.787529000	27.690410000	XXXX 1	xx	Pd	0.000
Pd70	1.959934000	1.394379000	26.202137000	XXXX 1	xx	Pd	0.000
Pd71	1.960153000	4.177870000	26.200896000	XXXX 1	xx	Pd	0.000
Pd72	1.960481000	6.962569000	26.201764000	XXXX 1	xx	Pd	0.000
Pd73	3.961758000	0.004018000	27.881437000	XXXX 1	xx	Pd	0.000
Pd74	3.961447000	2.788263000	27.880355000	XXXX 1	xx	Pd	0.000
Pd75	3.960674000	5.572141000	27.880094000	XXXX 1	xx	Pd	0.000
Pd76	6.005380000	1.394337000	26.271801000	XXXX 1	xx	Pd	0.000
Pd77	6.004791000	4.178256000	26.271219000	XXXX 1	xx	Pd	0.000
Pd78	6.004755000	6.963249000	26.271483000	XXXX 1	xx	Pd	0.000
H79	5.127259000	6.967639000	30.840284000	XXXX 1	xx	H	0.000
H80	4.821906000	2.786622000	26.297787000	XXXX 1	xx	H	0.000
H81	7.256914000	2.793149000	29.350546000	XXXX 1	xx	H	0.000
H82	4.821281000	0.002977000	26.298675000	XXXX 1	xx	H	0.000
H83	2.719338000	4.180047000	27.829845000	XXXX 1	xx	H	0.000
H84	2.775898000	6.968335000	30.875867000	XXXX 1	xx	H	0.000
H85	7.253666000	0.005944000	29.351004000	XXXX 1	xx	H	0.000
H86	2.717425000	6.966353000	27.832215000	XXXX 1	xx	H	0.000
H87	4.821717000	5.570828000	26.297796000	XXXX 1	xx	H	0.000
H88	2.717162000	1.396211000	27.832713000	XXXX 1	xx	H	0.000
H89	5.127101000	4.184105000	30.838566000	XXXX 1	xx	H	0.000
H90	5.127253000	1.400226000	30.841092000	XXXX 1	xx	H	0.000
H91	2.775515000	4.183993000	30.874512000	XXXX 1	xx	H	0.000
H92	2.776118000	1.399884000	30.876023000	XXXX 1	xx	H	0.000
H93	7.256923000	5.574752000	29.347557000	XXXX 1	xx	H	0.000

end

H_{r_i}/Pd(110) ($r_i = 1$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000

Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	4.020880000	8.351076000	24.905627000	XXXX	1	xx	Pd 0.000
Pd56	4.020694000	2.783435000	24.905387000	XXXX	1	xx	Pd 0.000
Pd57	4.020749000	5.567455000	24.905493000	XXXX	1	xx	Pd 0.000
Pd58	3.885331000	2.783236000	31.071378000	XXXX	1	xx	Pd 0.000
Pd59	3.948056000	8.351257000	28.221673000	XXXX	1	xx	Pd 0.000
Pd60	1.735095000	6.959361000	29.739393000	XXXX	1	xx	Pd 0.000
Pd61	6.003610000	1.391676000	29.706757000	XXXX	1	xx	Pd 0.000
Pd62	1.735349000	1.391300000	29.738120000	XXXX	1	xx	Pd 0.000
Pd63	3.885199000	8.350747000	31.071983000	XXXX	1	xx	Pd 0.000
Pd64	6.003597000	4.175296000	29.706247000	XXXX	1	xx	Pd 0.000
Pd65	1.735454000	4.175185000	29.737880000	XXXX	1	xx	Pd 0.000
Pd66	3.885224000	5.566956000	31.071638000	XXXX	1	xx	Pd 0.000
Pd67	7.871717000	5.567328000	28.115365000	XXXX	1	xx	Pd 0.000
Pd68	7.871539000	8.351544000	28.115910000	XXXX	1	xx	Pd 0.000
Pd69	7.871948000	2.783376000	28.114914000	XXXX	1	xx	Pd 0.000
Pd70	1.957303000	1.391172000	26.523874000	XXXX	1	xx	Pd 0.000
Pd71	1.957416000	4.175974000	26.523735000	XXXX	1	xx	Pd 0.000
Pd72	1.956908000	6.960003000	26.524344000	XXXX	1	xx	Pd 0.000
Pd73	3.948717000	2.783164000	28.220901000	XXXX	1	xx	Pd 0.000
Pd74	3.948190000	5.567453000	28.221357000	XXXX	1	xx	Pd 0.000
Pd75	6.003158000	6.959287000	29.706849000	XXXX	1	xx	Pd 0.000
Pd76	5.962440000	1.391156000	26.624856000	XXXX	1	xx	Pd 0.000
Pd77	5.962550000	4.175446000	26.624618000	XXXX	1	xx	Pd 0.000
Pd78	5.962502000	6.959487000	26.624939000	XXXX	1	xx	Pd 0.000
H79	5.048671000	6.958793000	31.265341000	XXXX	1	xx	H 0.000
H80	4.738683000	5.567414000	26.579677000	XXXX	1	xx	H 0.000
H81	5.048837000	1.391052000	31.265173000	XXXX	1	xx	H 0.000
H82	7.165949000	8.351349000	29.806732000	XXXX	1	xx	H 0.000
H83	2.724902000	4.174982000	28.234120000	XXXX	1	xx	H 0.000
H84	4.738494000	8.351134000	26.580100000	XXXX	1	xx	H 0.000
H85	5.048851000	4.174870000	31.264394000	XXXX	1	xx	H 0.000
H86	2.714568000	4.174805000	31.260064000	XXXX	1	xx	H 0.000
H87	2.724601000	1.391366000	28.234236000	XXXX	1	xx	H 0.000
H88	2.714635000	1.390986000	31.260341000	XXXX	1	xx	H 0.000
H89	4.739093000	2.783367000	26.579241000	XXXX	1	xx	H 0.000
H90	2.723944000	6.959110000	28.235444000	XXXX	1	xx	H 0.000
H91	2.714766000	6.958923000	31.261187000	XXXX	1	xx	H 0.000
H92	6.671796000	4.176639000	24.972607000	XXXX	1	xx	H 0.000
H93	6.671316000	1.392655000	24.972676000	XXXX	1	xx	H 0.000
H94	6.671186000	6.961309000	24.972665000	XXXX	1	xx	H 0.000

H95	7.166269000	5.567630000	29.805507000	XXXX	1	xx	H	0.000
H96	7.167702000	2.783480000	29.804541000	XXXX	1	xx	H	0.000
H97	2.828483000	4.175130000	24.902337000	XXXX	1	xx	H	0.000
H98	0.736509000	5.568065000	26.413481000	XXXX	1	xx	H	0.000
H99	2.827839000	6.958962000	24.902870000	XXXX	1	xx	H	0.000
H100	0.738427000	2.783680000	26.412342000	XXXX	1	xx	H	0.000
H101	2.828573000	1.390480000	24.902182000	XXXX	1	xx	H	0.000
H102	0.735045000	0.000056000	26.414758000	XXXX	1	xx	H	0.000

end

4. XYZ coordinates for the configurations in Fig. 2

H_{r_i}-N/Pd(110) ($r_i = 0.25$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)		
Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H	0.000
Pd55	3.937731000	8.350654000	24.800340000	XXXX	1	xx	Pd	0.000
Pd56	3.940191000	2.783815000	24.796769000	XXXX	1	xx	Pd	0.000
Pd57	3.937738000	5.570135000	24.799781000	XXXX	1	xx	Pd	0.000
Pd58	2.052149000	1.413960000	29.092799000	XXXX	1	xx	Pd	0.000
Pd59	2.051781000	4.149712000	29.092568000	XXXX	1	xx	Pd	0.000
Pd60	1.997360000	6.957223000	29.159257000	XXXX	1	xx	Pd	0.000
Pd61	0.030240000	0.005851000	30.615332000	XXXX	1	xx	Pd	0.000
Pd62	0.022053000	2.778909000	30.535942000	XXXX	1	xx	Pd	0.000

Pd63	0.026687000	5.553837000	30.614038000	XXXX 1	xx	Pd	0.000
Pd64	5.848954000	1.413581000	29.111733000	XXXX 1	xx	Pd	0.000
Pd65	5.847421000	4.149696000	29.111469000	XXXX 1	xx	Pd	0.000
Pd66	5.912919000	6.958398000	29.195459000	XXXX 1	xx	Pd	0.000
Pd67	7.875405000	8.357200000	27.686487000	XXXX 1	xx	Pd	0.000
Pd68	7.883763000	2.785382000	27.656454000	XXXX 1	xx	Pd	0.000
Pd69	7.874929000	5.562415000	27.685551000	XXXX 1	xx	Pd	0.000
Pd70	1.949969000	1.394584000	26.215836000	XXXX 1	xx	Pd	0.000
Pd71	1.949814000	4.173779000	26.215975000	XXXX 1	xx	Pd	0.000
Pd72	1.921416000	6.960336000	26.200408000	XXXX 1	xx	Pd	0.000
Pd73	3.955547000	0.023113000	27.619657000	XXXX 1	xx	Pd	0.000
Pd74	3.953996000	2.783165000	27.627066000	XXXX 1	xx	Pd	0.000
Pd75	3.955841000	5.543636000	27.619938000	XXXX 1	xx	Pd	0.000
Pd76	5.938423000	1.393127000	26.210687000	XXXX 1	xx	Pd	0.000
Pd77	5.938311000	4.175216000	26.210419000	XXXX 1	xx	Pd	0.000
Pd78	5.959992000	6.960257000	26.195051000	XXXX 1	xx	Pd	0.000
N79	3.956384000	6.959563000	28.988223000	XXXX 1	xx	N	0.000
H80	1.240323000	1.416690000	30.692787000	XXXX 1	xx	H	0.000
H81	1.236746000	4.142864000	30.691817000	XXXX 1	xx	H	0.000
H82	1.169344000	6.962767000	30.840379000	XXXX 1	xx	H	0.000
H83	6.689972000	1.404438000	30.694509000	XXXX 1	xx	H	0.000
H84	6.682951000	4.146220000	30.695422000	XXXX 1	xx	H	0.000
H85	6.766238000	6.955963000	30.845460000	XXXX 1	xx	H	0.000

end

H_{r_i}-N/Pd(110) ($r_i = 0.375$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000

H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.937500000	0.000525000	24.753379000	XXXX 1	xx	Pd	0.000
Pd56	3.947483000	2.781006000	24.779725000	XXXX 1	xx	Pd	0.000
Pd57	3.946744000	5.571453000	24.777989000	XXXX 1	xx	Pd	0.000
Pd58	2.257662000	1.381228000	29.235998000	XXXX 1	xx	Pd	0.000
Pd59	2.199957000	4.182381000	29.203876000	XXXX 1	xx	Pd	0.000
Pd60	2.269017000	6.986598000	29.243275000	XXXX 1	xx	Pd	0.000
Pd61	7.892933000	0.005741000	30.493332000	XXXX 1	xx	Pd	0.000
Pd62	0.024583000	2.780734000	30.512010000	XXXX 1	xx	Pd	0.000
Pd63	7.905482000	5.584422000	30.504272000	XXXX 1	xx	Pd	0.000
Pd64	5.601133000	1.365678000	29.298564000	XXXX 1	xx	Pd	0.000
Pd65	5.850655000	4.181058000	29.082610000	XXXX 1	xx	Pd	0.000
Pd66	5.639262000	7.007826000	29.245701000	XXXX 1	xx	Pd	0.000
Pd67	0.005183000	8.353922000	27.709711000	XXXX 1	xx	Pd	0.000
Pd68	-0.013029000	2.721010000	27.725426000	XXXX 1	xx	Pd	0.000
Pd69	7.866251000	5.631912000	27.718391000	XXXX 1	xx	Pd	0.000
Pd70	1.922415000	1.392269000	26.188110000	XXXX 1	xx	Pd	0.000
Pd71	1.940092000	4.176521000	26.160691000	XXXX 1	xx	Pd	0.000
Pd72	1.924003000	6.963617000	26.188039000	XXXX 1	xx	Pd	0.000
Pd73	3.943021000	0.004902000	27.444499000	XXXX 1	xx	Pd	0.000
Pd74	3.932948000	2.800838000	27.537483000	XXXX 1	xx	Pd	0.000
Pd75	3.930032000	5.557280000	27.535245000	XXXX 1	xx	Pd	0.000
Pd76	5.960486000	1.394940000	26.195792000	XXXX 1	xx	Pd	0.000
Pd77	5.962075000	4.176859000	26.193559000	XXXX 1	xx	Pd	0.000
Pd78	5.959968000	6.959455000	26.191523000	XXXX 1	xx	Pd	0.000
N79	3.868065000	8.369751000	29.405343000	XXXX 1	xx	N	0.000
H80	4.607071000	5.477162000	29.196275000	XXXX 1	xx	H	0.000
H81	1.189065000	1.400754000	30.706360000	XXXX 1	xx	H	0.000
H82	1.197854000	4.180234000	30.687300000	XXXX 1	xx	H	0.000
H83	1.194165000	6.964126000	30.702941000	XXXX 1	xx	H	0.000
H84	6.731758000	6.959916000	30.692466000	XXXX 1	xx	H	0.000
H85	6.729983000	4.185074000	30.646752000	XXXX 1	xx	H	0.000
H86	6.731435000	1.400336000	30.721556000	XXXX 1	xx	H	0.000
H87	1.108904000	4.172676000	27.775150000	XXXX 1	xx	H	0.000
H88	4.576773000	2.916822000	29.210746000	XXXX 1	xx	H	0.000

end

H_{r_i}-N/Pd(110) ($r_i = 0.5$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000

Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.921324000	8.342170000	24.781049000	XXXX	1	xx	Pd 0.000
Pd56	3.947635000	2.778541000	24.828705000	XXXX	1	xx	Pd 0.000
Pd57	3.947357000	5.550962000	24.827730000	XXXX	1	xx	Pd 0.000
Pd58	6.039866000	4.114250000	29.330683000	XXXX	1	xx	Pd 0.000
Pd59	1.627347000	6.904946000	29.538254000	XXXX	1	xx	Pd 0.000
Pd60	1.769937000	4.112429000	29.399971000	XXXX	1	xx	Pd 0.000
Pd61	6.235556000	1.304060000	29.521537000	XXXX	1	xx	Pd 0.000
Pd62	3.942869000	8.277683000	30.832029000	XXXX	1	xx	Pd 0.000
Pd63	3.947781000	2.701690000	30.755280000	XXXX	1	xx	Pd 0.000
Pd64	3.944625000	5.501603000	30.748839000	XXXX	1	xx	Pd 0.000
Pd65	1.615924000	1.326073000	29.552566000	XXXX	1	xx	Pd 0.000
Pd66	6.224918000	6.923749000	29.496866000	XXXX	1	xx	Pd 0.000
Pd67	3.963224000	8.318912000	28.044273000	XXXX	1	xx	Pd 0.000
Pd68	0.000249000	8.312598000	27.584753000	XXXX	1	xx	Pd 0.000
Pd69	7.893952000	2.760785000	27.670137000	XXXX	1	xx	Pd 0.000
Pd70	2.000324000	1.374207000	26.267654000	XXXX	1	xx	Pd 0.000
Pd71	1.994553000	4.154688000	26.253476000	XXXX	1	xx	Pd 0.000
Pd72	1.997593000	6.935737000	26.258962000	XXXX	1	xx	Pd 0.000
Pd73	0.018476000	5.508192000	27.666692000	XXXX	1	xx	Pd 0.000
Pd74	4.009431000	2.728285000	27.914014000	XXXX	1	xx	Pd 0.000
Pd75	4.009470000	5.551285000	27.911371000	XXXX	1	xx	Pd 0.000
Pd76	5.908935000	1.398322000	26.269676000	XXXX	1	xx	Pd 0.000
Pd77	5.889403000	4.153367000	26.284475000	XXXX	1	xx	Pd 0.000
Pd78	5.905098000	6.909740000	26.269298000	XXXX	1	xx	Pd 0.000
H79	7.322071000	2.830352000	29.381559000	XXXX	1	xx	H 0.000
H80	2.782321000	1.326800000	30.991378000	XXXX	1	xx	H 0.000
H81	5.110837000	1.322987000	30.993393000	XXXX	1	xx	H 0.000
H82	7.309248000	5.367405000	29.372911000	XXXX	1	xx	H 0.000
H83	5.128235000	4.102101000	30.902445000	XXXX	1	xx	H 0.000
H84	2.736872000	1.394970000	27.928765000	XXXX	1	xx	H 0.000
H85	2.780052000	6.873200000	30.985113000	XXXX	1	xx	H 0.000
H86	4.716361000	8.334486000	26.414874000	XXXX	1	xx	H 0.000
H87	2.796341000	4.134842000	27.901089000	XXXX	1	xx	H 0.000
H88	5.112121000	6.874220000	30.969249000	XXXX	1	xx	H 0.000

H89	2.749386000	6.891686000	27.899599000	XXXX 1	xx	H	0.000
H90	2.766829000	4.098545000	30.914980000	XXXX 1	xx	H	0.000
N91	7.876463000	8.280381000	29.556271000	XXXX 1	xx	N	0.000

end

H_{r_i}-N/Pd(110) ($r_i = 1$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	4.003708000	-0.000195000	24.897273000	XXXX 1	xx	Pd	0.000
Pd56	4.002111000	2.785547000	24.899743000	XXXX 1	xx	Pd	0.000
Pd57	3.904268000	5.570883000	25.064920000	XXXX 1	xx	Pd	0.000
Pd58	3.871533000	2.788583000	31.135740000	XXXX 1	xx	Pd	0.000
Pd59	3.940914000	0.016071000	28.292017000	XXXX 1	xx	Pd	0.000
Pd60	1.689564000	6.962333000	29.747010000	XXXX 1	xx	Pd	0.000
Pd61	6.167909000	1.423212000	29.880899000	XXXX 1	xx	Pd	0.000
Pd62	1.577208000	1.400234000	29.866717000	XXXX 1	xx	Pd	0.000

Pd63	3.863159000	0.009165000	31.084006000	XXXX	1	xx	Pd 0.000
Pd64	6.169100000	4.145169000	29.882108000	XXXX	1	xx	Pd 0.000
Pd65	1.565448000	4.170276000	29.880902000	XXXX	1	xx	Pd 0.000
Pd66	3.862290000	5.562428000	31.103680000	XXXX	1	xx	Pd 0.000
Pd67	-0.051126000	5.582532000	28.080323000	XXXX	1	xx	Pd 0.000
Pd68	7.824707000	8.343898000	28.075461000	XXXX	1	xx	Pd 0.000
Pd69	7.809028000	2.776142000	27.963972000	XXXX	1	xx	Pd 0.000
Pd70	2.022405000	1.384641000	26.581171000	XXXX	1	xx	Pd 0.000
Pd71	1.985456000	4.172277000	26.617893000	XXXX	1	xx	Pd 0.000
Pd72	1.939336000	6.967173000	26.579649000	XXXX	1	xx	Pd 0.000
Pd73	3.963768000	2.781367000	28.335381000	XXXX	1	xx	Pd 0.000
Pd74	3.919869000	5.548594000	28.323663000	XXXX	1	xx	Pd 0.000
Pd75	5.970531000	6.960179000	29.695448000	XXXX	1	xx	Pd 0.000
Pd76	5.880600000	1.390382000	26.597993000	XXXX	1	xx	Pd 0.000
Pd77	5.891816000	4.172675000	26.612977000	XXXX	1	xx	Pd 0.000
Pd78	5.913577000	6.966196000	26.625469000	XXXX	1	xx	Pd 0.000
H79	5.028141000	6.964491000	31.244543000	XXXX	1	xx	H 0.000
H80	4.713341000	5.575819000	26.707661000	XXXX	1	xx	H 0.000
H81	5.022513000	1.383216000	31.317874000	XXXX	1	xx	H 0.000
H82	-0.657696000	5.676084000	29.805557000	XXXX	1	xx	H 0.000
H83	2.723137000	4.150020000	28.356225000	XXXX	1	xx	H 0.000
H84	4.650364000	-0.010234000	26.605472000	XXXX	1	xx	H 0.000
H85	5.024871000	4.188441000	31.320515000	XXXX	1	xx	H 0.000
H86	2.707803000	4.182998000	31.314539000	XXXX	1	xx	H 0.000
H87	2.731486000	1.402439000	28.340124000	XXXX	1	xx	H 0.000
H88	2.708973000	1.389985000	31.306676000	XXXX	1	xx	H 0.000
H89	4.629793000	2.785328000	26.629219000	XXXX	1	xx	H 0.000
H90	2.729685000	6.970486000	28.278242000	XXXX	1	xx	H 0.000
H91	2.690258000	6.963139000	31.243406000	XXXX	1	xx	H 0.000
H92	6.679879000	4.176414000	25.003158000	XXXX	1	xx	H 0.000
H93	6.668363000	1.390353000	24.987417000	XXXX	1	xx	H 0.000
H94	6.680672000	6.962414000	24.995212000	XXXX	1	xx	H 0.000
H95	7.214158000	8.245211000	29.800198000	XXXX	1	xx	H 0.000
H96	2.754409000	4.116442000	24.931511000	XXXX	1	xx	H 0.000
H97	0.755818000	5.546053000	26.405725000	XXXX	1	xx	H 0.000
H98	2.751232000	7.026322000	24.928501000	XXXX	1	xx	H 0.000
H99	4.765655000	5.567570000	23.511258000	XXXX	1	xx	H 0.000
H100	0.853129000	2.764244000	26.295540000	XXXX	1	xx	H 0.000
H101	2.814243000	1.392596000	24.908668000	XXXX	1	xx	H 0.000
H102	0.756815000	8.391391000	26.409586000	XXXX	1	xx	H 0.000
N103	7.809180000	2.781529000	29.958527000	XXXX	1	xx	N 0.000
end							

H_{r_i}-NH/Pd(110) ($r_i = 0.25$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000

Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784472000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784352000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784497000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083100000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082979000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082862000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883688000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883508000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883805000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056688000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056864000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056564000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.925726000	8.349452000	24.787019000	XXXX 1	xx	Pd	0.000
Pd56	3.926170000	2.787210000	24.787024000	XXXX 1	xx	Pd	0.000
Pd57	3.933285000	5.568290000	24.787863000	XXXX 1	xx	Pd	0.000
Pd58	2.030628000	6.977798000	29.103923000	XXXX 1	xx	Pd	0.000
Pd59	2.090103000	1.395074000	29.045028000	XXXX 1	xx	Pd	0.000
Pd60	2.030788000	4.164419000	29.103897000	XXXX 1	xx	Pd	0.000
Pd61	7.790035000	5.573261000	30.516000000	XXXX 1	xx	Pd	0.000
Pd62	7.814793000	8.331515000	30.527490000	XXXX 1	xx	Pd	0.000
Pd63	7.815050000	2.813604000	30.527598000	XXXX 1	xx	Pd	0.000
Pd64	5.831274000	1.395024000	29.041339000	XXXX 1	xx	Pd	0.000
Pd65	5.783770000	4.168669000	29.083821000	XXXX 1	xx	Pd	0.000
Pd66	5.783617000	6.974044000	29.083980000	XXXX 1	xx	Pd	0.000
Pd67	7.849084000	8.351175000	27.641046000	XXXX 1	xx	Pd	0.000
Pd68	7.849160000	2.787365000	27.640919000	XXXX 1	xx	Pd	0.000
Pd69	7.859172000	5.569464000	27.656765000	XXXX 1	xx	Pd	0.000
Pd70	1.939609000	1.393114000	26.212870000	XXXX 1	xx	Pd	0.000
Pd71	1.937923000	4.173545000	26.212740000	XXXX 1	xx	Pd	0.000
Pd72	1.937647000	6.964250000	26.212239000	XXXX 1	xx	Pd	0.000
Pd73	3.944000000	8.357410000	27.601746000	XXXX 1	xx	Pd	0.000
Pd74	3.943733000	2.782760000	27.602321000	XXXX 1	xx	Pd	0.000
Pd75	3.945724000	5.570879000	27.596134000	XXXX 1	xx	Pd	0.000
Pd76	5.914332000	1.392811000	26.172981000	XXXX 1	xx	Pd	0.000
Pd77	5.922336000	4.177281000	26.192779000	XXXX 1	xx	Pd	0.000
Pd78	5.923858000	6.961240000	26.190085000	XXXX 1	xx	Pd	0.000
N79	1.317611000	1.397892000	30.882450000	XXXX 1	xx	N	0.000
H80	1.958971000	1.396849000	31.690554000	XXXX 1	xx	H	0.000
H81	3.177778000	5.571400000	29.215151000	XXXX 1	xx	H	0.000
H82	1.130548000	6.889019000	30.656603000	XXXX 1	xx	H	0.000
H83	1.131219000	4.257537000	30.657519000	XXXX 1	xx	H	0.000
H84	-1.322012000	4.131936000	30.662973000	XXXX 1	xx	H	0.000
H85	6.553088000	7.014823000	30.663330000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH/Pd(110) ($r_i = 0.375$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000

Pd3	5.905756000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX	1	xx	Pd 0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX	1	xx	Pd 0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784472000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784352000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784497000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083100000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082979000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082862000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883688000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883508000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883805000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056688000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056864000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056564000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.936384000	8.351879000	24.795597000	XXXX	1	xx	Pd 0.000
Pd56	3.927788000	2.781059000	24.808279000	XXXX	1	xx	Pd 0.000
Pd57	3.936783000	5.564805000	24.795488000	XXXX	1	xx	Pd 0.000
Pd58	2.027672000	1.397610000	29.151537000	XXXX	1	xx	Pd 0.000
Pd59	2.026495000	4.157961000	29.151283000	XXXX	1	xx	Pd 0.000
Pd60	2.026345000	6.954042000	29.160652000	XXXX	1	xx	Pd 0.000
Pd61	7.852838000	8.350924000	30.659753000	XXXX	1	xx	Pd 0.000
Pd62	0.021094000	2.774159000	30.604337000	XXXX	1	xx	Pd 0.000
Pd63	7.855261000	5.548670000	30.659128000	XXXX	1	xx	Pd 0.000
Pd64	5.841970000	1.372266000	29.133103000	XXXX	1	xx	Pd 0.000
Pd65	5.842335000	4.183799000	29.134196000	XXXX	1	xx	Pd 0.000
Pd66	5.787536000	6.954335000	29.036792000	XXXX	1	xx	Pd 0.000
Pd67	0.009963000	8.349035000	27.672350000	XXXX	1	xx	Pd 0.000
Pd68	7.863547000	2.779614000	27.696790000	XXXX	1	xx	Pd 0.000
Pd69	0.009649000	5.561689000	27.672609000	XXXX	1	xx	Pd 0.000
Pd70	1.930510000	1.390107000	26.220440000	XXXX	1	xx	Pd 0.000
Pd71	1.930491000	4.171067000	26.220946000	XXXX	1	xx	Pd 0.000

Pd72	1.942547000	6.957189000	26.207291000	XXXX 1	xx	Pd	0.000
Pd73	3.932904000	8.355682000	27.597629000	XXXX 1	xx	Pd	0.000
Pd74	3.907458000	2.779111000	27.631881000	XXXX 1	xx	Pd	0.000
Pd75	3.933295000	5.553685000	27.598559000	XXXX 1	xx	Pd	0.000
Pd76	5.931613000	1.388530000	26.217356000	XXXX 1	xx	Pd	0.000
Pd77	5.931919000	4.171028000	26.217085000	XXXX 1	xx	Pd	0.000
Pd78	5.933071000	6.955904000	26.221341000	XXXX 1	xx	Pd	0.000
N79	6.402194000	6.947930000	30.923349000	XXXX 1	xx	N	0.000
H80	1.219173000	1.317799000	30.743348000	XXXX 1	xx	H	0.000
H81	3.181821000	8.368122000	29.229584000	XXXX 1	xx	H	0.000
H82	6.690213000	1.435585000	30.739222000	XXXX 1	xx	H	0.000
H83	4.688731000	2.778123000	29.243130000	XXXX 1	xx	H	0.000
H84	5.695299000	6.944211000	31.676065000	XXXX 1	xx	H	0.000
H85	3.181401000	5.539323000	29.229882000	XXXX 1	xx	H	0.000
H86	6.691053000	4.110808000	30.739860000	XXXX 1	xx	H	0.000
H87	1.220466000	4.227845000	30.744272000	XXXX 1	xx	H	0.000
H88	1.251673000	6.949708000	30.765639000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH/Pd(110) ($r_i = 0.5$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000

H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.929526000	8.350637000	24.805141000	XXXX 1	xx	Pd	0.000
Pd56	3.924454000	2.783381000	24.801541000	XXXX 1	xx	Pd	0.000
Pd57	3.930144000	5.568470000	24.805193000	XXXX 1	xx	Pd	0.000
Pd58	1.821308000	4.158414000	29.220533000	XXXX 1	xx	Pd	0.000
Pd59	1.791009000	6.955836000	29.262756000	XXXX 1	xx	Pd	0.000
Pd60	1.821435000	1.402593000	29.220810000	XXXX 1	xx	Pd	0.000
Pd61	6.101897000	4.207441000	29.333725000	XXXX 1	xx	Pd	0.000
Pd62	6.312352000	6.956425000	29.310317000	XXXX 1	xx	Pd	0.000
Pd63	6.102840000	1.353582000	29.333559000	XXXX 1	xx	Pd	0.000
Pd64	3.910721000	8.355922000	30.710468000	XXXX 1	xx	Pd	0.000
Pd65	3.883328000	2.777640000	30.645954000	XXXX 1	xx	Pd	0.000
Pd66	3.910185000	5.554018000	30.711375000	XXXX 1	xx	Pd	0.000
Pd67	7.877598000	5.547442000	27.574813000	XXXX 1	xx	Pd	0.000
Pd68	7.877430000	0.015879000	27.574105000	XXXX 1	xx	Pd	0.000
Pd69	0.023067000	2.781545000	27.621513000	XXXX 1	xx	Pd	0.000
Pd70	1.979940000	1.389850000	26.216218000	XXXX 1	xx	Pd	0.000
Pd71	1.979815000	4.175562000	26.216164000	XXXX 1	xx	Pd	0.000
Pd72	1.976671000	6.959131000	26.223812000	XXXX 1	xx	Pd	0.000
Pd73	3.872989000	8.345760000	27.787875000	XXXX 1	xx	Pd	0.000
Pd74	3.873384000	2.781275000	27.776181000	XXXX 1	xx	Pd	0.000
Pd75	3.872301000	5.569989000	27.788259000	XXXX 1	xx	Pd	0.000
Pd76	5.899258000	1.393407000	26.199208000	XXXX 1	xx	Pd	0.000
Pd77	5.899716000	4.172658000	26.198843000	XXXX 1	xx	Pd	0.000
Pd78	5.896626000	6.958731000	26.206958000	XXXX 1	xx	Pd	0.000
H79	7.257832000	2.779412000	29.282386000	XXXX 1	xx	H	0.000
H80	2.677747000	4.223468000	30.781166000	XXXX 1	xx	H	0.000
H81	5.894993000	6.952551000	31.936692000	XXXX 1	xx	H	0.000
H82	5.083622000	4.178134000	27.803651000	XXXX 1	xx	H	0.000
H83	2.678953000	1.332020000	30.780026000	XXXX 1	xx	H	0.000
H84	0.649236000	5.535530000	29.281110000	XXXX 1	xx	H	0.000
H85	2.645194000	6.954588000	30.834557000	XXXX 1	xx	H	0.000
H86	5.066884000	4.108042000	30.848633000	XXXX 1	xx	H	0.000
H87	5.066901000	1.448403000	30.848423000	XXXX 1	xx	H	0.000
H88	0.648329000	0.024617000	29.281112000	XXXX 1	xx	H	0.000
H89	5.083943000	1.384257000	27.803894000	XXXX 1	xx	H	0.000
H90	5.087377000	6.956793000	27.821969000	XXXX 1	xx	H	0.000
N91	5.337701000	6.952328000	31.065809000	XXXX 1	xx	N	0.000

end

H_{r_i}-NH/Pd(110) $(r_i = 1)$

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000

Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	4.018123000	8.340731000	24.895961000	XXXX	1	xx	Pd 0.000
Pd56	4.022707000	2.772673000	24.900828000	XXXX	1	xx	Pd 0.000
Pd57	4.022531000	5.556774000	24.900840000	XXXX	1	xx	Pd 0.000
Pd58	3.909905000	2.710159000	31.165121000	XXXX	1	xx	Pd 0.000
Pd59	3.939691000	8.309775000	28.233960000	XXXX	1	xx	Pd 0.000
Pd60	1.730445000	6.906294000	29.756034000	XXXX	1	xx	Pd 0.000
Pd61	5.992543000	1.341161000	29.677715000	XXXX	1	xx	Pd 0.000
Pd62	1.732516000	1.352100000	29.758985000	XXXX	1	xx	Pd 0.000
Pd63	3.931413000	8.288883000	31.087484000	XXXX	1	xx	Pd 0.000
Pd64	6.018440000	4.120743000	29.692819000	XXXX	1	xx	Pd 0.000
Pd65	1.610908000	4.130436000	29.763752000	XXXX	1	xx	Pd 0.000
Pd66	3.905736000	5.515264000	31.164260000	XXXX	1	xx	Pd 0.000
Pd67	7.865645000	5.536648000	28.068788000	XXXX	1	xx	Pd 0.000
Pd68	7.874998000	8.310782000	28.115810000	XXXX	1	xx	Pd 0.000
Pd69	7.865965000	2.732106000	28.070224000	XXXX	1	xx	Pd 0.000
Pd70	1.974265000	1.363089000	26.527047000	XXXX	1	xx	Pd 0.000
Pd71	1.966915000	4.149647000	26.521294000	XXXX	1	xx	Pd 0.000
Pd72	1.972677000	6.936686000	26.525889000	XXXX	1	xx	Pd 0.000
Pd73	3.926377000	2.747641000	28.241326000	XXXX	1	xx	Pd 0.000
Pd74	3.926044000	5.520148000	28.239529000	XXXX	1	xx	Pd 0.000
Pd75	5.992755000	6.898596000	29.676892000	XXXX	1	xx	Pd 0.000
Pd76	5.940210000	1.362859000	26.617765000	XXXX	1	xx	Pd 0.000
Pd77	5.938882000	4.147109000	26.618402000	XXXX	1	xx	Pd 0.000
Pd78	5.940858000	6.932472000	26.617879000	XXXX	1	xx	Pd 0.000
H79	4.696514000	5.538260000	26.595735000	XXXX	1	xx	H 0.000
H80	2.714470000	4.130131000	28.199651000	XXXX	1	xx	H 0.000
H81	4.704844000	8.321082000	26.579712000	XXXX	1	xx	H 0.000
H82	2.710559000	1.345267000	28.252621000	XXXX	1	xx	H 0.000
H83	4.695023000	2.751968000	26.596721000	XXXX	1	xx	H 0.000
H84	2.710846000	6.915594000	28.249816000	XXXX	1	xx	H 0.000
H85	6.669280000	4.176193000	24.978395000	XXXX	1	xx	H 0.000
H86	6.669067000	1.393065000	24.978047000	XXXX	1	xx	H 0.000
H87	6.669167000	6.959805000	24.977986000	XXXX	1	xx	H 0.000
H88	2.834616000	4.164592000	24.895985000	XXXX	1	xx	H 0.000
H89	0.762628000	5.547479000	26.391529000	XXXX	1	xx	H 0.000
H90	2.828361000	6.946772000	24.899483000	XXXX	1	xx	H 0.000

H91	0.762961000	2.752537000	26.391966000	XXXX 1	xx	H	0.000
H92	2.828792000	1.383117000	24.899330000	XXXX 1	xx	H	0.000
H93	0.760588000	8.327767000	26.396882000	XXXX 1	xx	H	0.000
H94	2.748540000	1.272514000	31.271898000	XXXX 1	xx	H	0.000
H95	2.744969000	6.950699000	31.268694000	XXXX 1	xx	H	0.000
H96	7.162064000	8.292114000	29.780604000	XXXX 1	xx	H	0.000
H97	5.111666000	6.853771000	31.254292000	XXXX 1	xx	H	0.000
H98	7.150845000	2.717272000	29.769204000	XXXX 1	xx	H	0.000
H99	5.155412000	4.113115000	31.258755000	XXXX 1	xx	H	0.000
H100	1.959475000	4.105465000	32.454506000	XXXX 1	xx	H	0.000
H101	5.114926000	1.366260000	31.256560000	XXXX 1	xx	H	0.000
H102	7.153191000	5.517182000	29.768043000	XXXX 1	xx	H	0.000
N103	2.500450000	4.109571000	31.572556000	XXXX 1	xx	N	0.000
end							

H_{r_i}-NH_2/Pd(110) ($r_i = 0.25$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784472000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784352000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784497000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083100000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082979000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082862000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883688000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883508000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883805000	6.960290000	16.147130000	XXXX 1	xx	H	0.000

H52	7.056688000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056864000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056564000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.930696000	8.354159000	24.805257000	XXXX 1	xx	Pd	0.000
Pd56	3.929680000	2.783749000	24.798558000	XXXX 1	xx	Pd	0.000
Pd57	3.929947000	5.572079000	24.798546000	XXXX 1	xx	Pd	0.000
Pd58	3.933520000	2.838094000	30.492131000	XXXX 1	xx	Pd	0.000
Pd59	5.987151000	4.190903000	29.050613000	XXXX 1	xx	Pd	0.000
Pd60	6.021582000	6.975276000	29.112017000	XXXX 1	xx	Pd	0.000
Pd61	3.927138000	0.024761000	30.512340000	XXXX 1	xx	Pd	0.000
Pd62	1.849041000	1.411805000	29.110788000	XXXX 1	xx	Pd	0.000
Pd63	3.933664000	5.565106000	30.486474000	XXXX 1	xx	Pd	0.000
Pd64	1.849300000	6.971642000	29.109881000	XXXX 1	xx	Pd	0.000
Pd65	6.022066000	1.406535000	29.111499000	XXXX 1	xx	Pd	0.000
Pd66	1.866341000	4.191549000	29.065771000	XXXX 1	xx	Pd	0.000
Pd67	7.866667000	0.010869000	27.617323000	XXXX 1	xx	Pd	0.000
Pd68	7.868882000	2.796774000	27.619035000	XXXX 1	xx	Pd	0.000
Pd69	-0.005439000	5.576758000	27.619652000	XXXX 1	xx	Pd	0.000
Pd70	1.972441000	1.397904000	26.229204000	XXXX 1	xx	Pd	0.000
Pd71	1.977528000	4.180997000	26.211333000	XXXX 1	xx	Pd	0.000
Pd72	1.972169000	6.964100000	26.228535000	XXXX 1	xx	Pd	0.000
Pd73	3.938896000	8.360077000	27.690997000	XXXX 1	xx	Pd	0.000
Pd74	3.928375000	2.783678000	27.695294000	XXXX 1	xx	Pd	0.000
Pd75	3.928076000	5.585112000	27.693385000	XXXX 1	xx	Pd	0.000
Pd76	5.891821000	1.398952000	26.221115000	XXXX 1	xx	Pd	0.000
Pd77	5.885311000	4.180275000	26.203511000	XXXX 1	xx	Pd	0.000
Pd78	5.892237000	6.962124000	26.220448000	XXXX 1	xx	Pd	0.000
N79	4.318132000	4.205270000	32.023586000	XXXX 1	xx	N	0.000
H80	5.136811000	6.984337000	30.659174000	XXXX 1	xx	H	0.000
H81	5.138997000	1.422695000	30.658760000	XXXX 1	xx	H	0.000
H82	2.708585000	1.398256000	30.658568000	XXXX 1	xx	H	0.000
H83	3.634428000	4.205653000	32.789156000	XXXX 1	xx	H	0.000
H84	5.273152000	4.207520000	32.398584000	XXXX 1	xx	H	0.000
H85	2.707127000	7.011319000	30.658555000	XXXX 1	xx	H	0.000
end							

H_{r_i}-NH_2/Pd(110) ($r_i = 0.375$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000

Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.937483000	8.352332000	24.782980000	XXXX 1	xx	Pd	0.000
Pd56	3.939098000	2.788260000	24.792720000	XXXX 1	xx	Pd	0.000
Pd57	3.938360000	5.565254000	24.804044000	XXXX 1	xx	Pd	0.000
Pd58	1.770765000	4.165239000	29.161879000	XXXX 1	xx	Pd	0.000
Pd59	1.865001000	6.960465000	29.089801000	XXXX 1	xx	Pd	0.000
Pd60	1.885828000	1.390308000	29.034685000	XXXX 1	xx	Pd	0.000
Pd61	5.999997000	1.390204000	29.035761000	XXXX 1	xx	Pd	0.000
Pd62	6.126302000	4.164536000	29.171331000	XXXX 1	xx	Pd	0.000
Pd63	6.020621000	6.960691000	29.091343000	XXXX 1	xx	Pd	0.000
Pd64	3.943420000	-0.000300000	30.474792000	XXXX 1	xx	Pd	0.000
Pd65	3.945221000	2.785424000	30.500653000	XXXX 1	xx	Pd	0.000
Pd66	3.944260000	5.567872000	30.519721000	XXXX 1	xx	Pd	0.000
Pd67	0.004751000	2.780478000	27.561641000	XXXX 1	xx	Pd	0.000
Pd68	0.002679000	5.561272000	27.552169000	XXXX 1	xx	Pd	0.000
Pd69	0.003684000	0.011675000	27.565458000	XXXX 1	xx	Pd	0.000
Pd70	1.982831000	1.395811000	26.182176000	XXXX 1	xx	Pd	0.000
Pd71	1.996464000	4.173974000	26.217941000	XXXX 1	xx	Pd	0.000
Pd72	1.991889000	6.955372000	26.195554000	XXXX 1	xx	Pd	0.000
Pd73	3.942235000	8.347797000	27.635384000	XXXX 1	xx	Pd	0.000
Pd74	3.944272000	2.796228000	27.687420000	XXXX 1	xx	Pd	0.000
Pd75	3.944553000	5.546060000	27.714551000	XXXX 1	xx	Pd	0.000
Pd76	5.894478000	1.396316000	26.180087000	XXXX 1	xx	Pd	0.000
Pd77	5.885027000	4.173987000	26.216323000	XXXX 1	xx	Pd	0.000
Pd78	5.885961000	6.955768000	26.193263000	XXXX 1	xx	Pd	0.000
H79	2.741625000	1.380142000	30.603025000	XXXX 1	xx	H	0.000
H80	2.771500000	4.174013000	30.665981000	XXXX 1	xx	H	0.000
H81	5.147352000	1.378625000	30.602546000	XXXX 1	xx	H	0.000
H82	0.004140000	7.024024000	28.895593000	XXXX 1	xx	H	0.000
H83	5.135486000	6.979394000	30.654304000	XXXX 1	xx	H	0.000
H84	0.018973000	3.229136000	30.897625000	XXXX 1	xx	H	0.000
H85	5.115935000	4.174034000	30.669079000	XXXX 1	xx	H	0.000
H86	0.017874000	4.884739000	30.999794000	XXXX 1	xx	H	0.000
N87	0.016531000	4.095154000	30.341650000	XXXX 1	xx	N	0.000
H88	2.753630000	6.977783000	30.655248000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH_2/Pd(110) ($r_i = 0.5$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000

Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.925275000	0.000583000	24.788301000	XXXX	1	xx	Pd 0.000
Pd56	3.930306000	2.790112000	24.798702000	XXXX	1	xx	Pd 0.000
Pd57	3.930304000	5.563296000	24.799603000	XXXX	1	xx	Pd 0.000
Pd58	1.754506000	4.178137000	29.197052000	XXXX	1	xx	Pd 0.000
Pd59	1.855692000	6.955815000	29.125534000	XXXX	1	xx	Pd 0.000
Pd60	1.856068000	1.397755000	29.125185000	XXXX	1	xx	Pd 0.000
Pd61	6.097474000	1.394656000	29.263098000	XXXX	1	xx	Pd 0.000
Pd62	6.123257000	4.177648000	29.225524000	XXXX	1	xx	Pd 0.000
Pd63	6.100192000	6.961945000	29.265858000	XXXX	1	xx	Pd 0.000
Pd64	3.918235000	0.005904000	30.549279000	XXXX	1	xx	Pd 0.000
Pd65	3.927958000	2.790280000	30.551503000	XXXX	1	xx	Pd 0.000
Pd66	3.927888000	5.570131000	30.553126000	XXXX	1	xx	Pd 0.000
Pd67	7.867088000	2.797858000	27.565011000	XXXX	1	xx	Pd 0.000
Pd68	7.867424000	5.557868000	27.567628000	XXXX	1	xx	Pd 0.000
Pd69	7.871551000	0.001687000	27.573563000	XXXX	1	xx	Pd 0.000
Pd70	1.973398000	1.402262000	26.194542000	XXXX	1	xx	Pd 0.000
Pd71	1.973162000	4.177430000	26.207595000	XXXX	1	xx	Pd 0.000
Pd72	1.973047000	6.952148000	26.194780000	XXXX	1	xx	Pd 0.000
Pd73	3.882511000	0.000635000	27.690349000	XXXX	1	xx	Pd 0.000
Pd74	3.903113000	2.826372000	27.727793000	XXXX	1	xx	Pd 0.000

Pd75	3.902995000	5.528517000	27.731015000	XXXX 1	xx	Pd	0.000
Pd76	5.906997000	1.400965000	26.164596000	XXXX 1	xx	Pd	0.000
Pd77	5.880552000	4.177344000	26.217658000	XXXX 1	xx	Pd	0.000
Pd78	5.906616000	6.953099000	26.166132000	XXXX 1	xx	Pd	0.000
H79	2.737390000	1.391015000	30.697324000	XXXX 1	xx	H	0.000
H80	2.759253000	4.182571000	30.702859000	XXXX 1	xx	H	0.000
H81	5.083034000	1.382630000	30.767007000	XXXX 1	xx	H	0.000
H82	0.040920000	6.967304000	28.891539000	XXXX 1	xx	H	0.000
H83	5.083797000	6.980956000	30.768425000	XXXX 1	xx	H	0.000
H84	0.022558000	3.313948000	30.997350000	XXXX 1	xx	H	0.000
H85	5.098577000	4.181967000	30.716971000	XXXX 1	xx	H	0.000
H86	0.021621000	4.973243000	31.034888000	XXXX 1	xx	H	0.000
H87	0.040648000	1.387571000	28.888217000	XXXX 1	xx	H	0.000
N88	0.013820000	4.157484000	30.402532000	XXXX 1	xx	N	0.000
H89	5.060679000	6.943622000	27.746447000	XXXX 1	xx	H	0.000
H90	2.737240000	6.972107000	30.698850000	XXXX 1	xx	H	0.000
H91	5.059265000	1.410625000	27.745142000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH_2/Pd(110) ($r_i = 1$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000

H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	4.013665000	-0.000748000	24.885890000	XXXX 1	xx	Pd	0.000
Pd56	4.010226000	2.785910000	24.885896000	XXXX 1	xx	Pd	0.000
Pd57	4.005853000	5.563042000	24.894063000	XXXX 1	xx	Pd	0.000
Pd58	3.878718000	2.782057000	31.086004000	XXXX 1	xx	Pd	0.000
Pd59	3.964010000	0.003721000	28.196204000	XXXX 1	xx	Pd	0.000
Pd60	1.721917000	6.959017000	29.732703000	XXXX 1	xx	Pd	0.000
Pd61	5.999116000	1.387218000	29.662123000	XXXX 1	xx	Pd	0.000
Pd62	1.730360000	1.388163000	29.710149000	XXXX 1	xx	Pd	0.000
Pd63	3.889406000	8.350391000	31.039333000	XXXX 1	xx	Pd	0.000
Pd64	6.081637000	4.170334000	29.771253000	XXXX 1	xx	Pd	0.000
Pd65	1.622336000	4.167990000	29.806434000	XXXX 1	xx	Pd	0.000
Pd66	3.876172000	5.566568000	31.114343000	XXXX 1	xx	Pd	0.000
Pd67	7.806326000	5.548237000	28.053791000	XXXX 1	xx	Pd	0.000
Pd68	7.804087000	8.347899000	28.047043000	XXXX 1	xx	Pd	0.000
Pd69	7.798465000	2.794522000	28.039457000	XXXX 1	xx	Pd	0.000
Pd70	1.946106000	1.391921000	26.508288000	XXXX 1	xx	Pd	0.000
Pd71	1.982991000	4.173813000	26.569754000	XXXX 1	xx	Pd	0.000
Pd72	1.961591000	6.954287000	26.523976000	XXXX 1	xx	Pd	0.000
Pd73	3.983524000	2.783689000	28.248119000	XXXX 1	xx	Pd	0.000
Pd74	3.957829000	5.554569000	28.297548000	XXXX 1	xx	Pd	0.000
Pd75	6.006706000	6.954931000	29.693362000	XXXX 1	xx	Pd	0.000
Pd76	5.999428000	1.396746000	26.426296000	XXXX 1	xx	Pd	0.000
Pd77	5.908703000	4.174734000	26.581864000	XXXX 1	xx	Pd	0.000
Pd78	5.905351000	6.949699000	26.589267000	XXXX 1	xx	Pd	0.000
H79	5.052691000	6.967123000	31.241983000	XXXX 1	xx	H	0.000
H80	4.642990000	5.549992000	26.614731000	XXXX 1	xx	H	0.000
H81	5.063277000	1.383082000	31.209219000	XXXX 1	xx	H	0.000
H82	7.791626000	6.941475000	29.416531000	XXXX 1	xx	H	0.000
H83	2.721561000	4.159275000	28.353911000	XXXX 1	xx	H	0.000
H84	4.749068000	0.066609000	26.563077000	XXXX 1	xx	H	0.000
H85	5.041631000	4.174225000	31.263617000	XXXX 1	xx	H	0.000
H86	2.702447000	4.172865000	31.267750000	XXXX 1	xx	H	0.000
H87	2.753137000	1.387927000	28.158016000	XXXX 1	xx	H	0.000
H88	2.727280000	1.372315000	31.241231000	XXXX 1	xx	H	0.000
H89	4.724657000	2.718905000	26.583164000	XXXX 1	xx	H	0.000
H90	2.748376000	6.979053000	28.180609000	XXXX 1	xx	H	0.000
H91	2.726557000	6.979336000	31.263858000	XXXX 1	xx	H	0.000
H92	6.681240000	4.160025000	24.972723000	XXXX 1	xx	H	0.000
H93	6.679590000	6.977390000	24.973220000	XXXX 1	xx	H	0.000
H94	7.791181000	1.402999000	29.406363000	XXXX 1	xx	H	0.000
H95	2.790730000	4.174447000	24.920175000	XXXX 1	xx	H	0.000
H96	0.742164000	5.537922000	26.406023000	XXXX 1	xx	H	0.000
H97	2.817300000	6.955600000	24.905077000	XXXX 1	xx	H	0.000
H98	0.729722000	2.813433000	26.388211000	XXXX 1	xx	H	0.000
H99	2.822802000	1.394523000	24.904217000	XXXX 1	xx	H	0.000
H100	0.719901000	8.348192000	26.382081000	XXXX 1	xx	H	0.000
H101	7.712108000	3.265829000	31.616032000	XXXX 1	xx	H	0.000
H102	7.711569000	4.919896000	31.696989000	XXXX 1	xx	H	0.000
N103	7.764777000	4.124515000	31.045209000	XXXX 1	xx	N	0.000

end

H_{r_i}-NH_3/Pd(110) ($r_i = 0.25$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000

Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.940356000	-0.000203000	24.803970000	XXXX	1	xx	Pd 0.000
Pd56	3.939185000	2.782493000	24.803717000	XXXX	1	xx	Pd 0.000
Pd57	3.941989000	5.567510000	24.803341000	XXXX	1	xx	Pd 0.000
Pd58	1.886805000	6.958514000	29.084376000	XXXX	1	xx	Pd 0.000
Pd59	3.937575000	0.001271000	27.670955000	XXXX	1	xx	Pd 0.000
Pd60	6.012429000	4.171339000	29.106757000	XXXX	1	xx	Pd 0.000
Pd61	5.984080000	1.390546000	29.085399000	XXXX	1	xx	Pd 0.000
Pd62	6.012243000	6.962824000	29.110490000	XXXX	1	xx	Pd 0.000
Pd63	3.884895000	5.564282000	30.472928000	XXXX	1	xx	Pd 0.000
Pd64	3.945216000	5.567859000	27.692877000	XXXX	1	xx	Pd 0.000
Pd65	0.002831000	5.567377000	27.645727000	XXXX	1	xx	Pd 0.000
Pd66	3.936234000	2.780231000	27.665007000	XXXX	1	xx	Pd 0.000
Pd67	-0.000652000	2.779833000	27.637509000	XXXX	1	xx	Pd 0.000
Pd68	1.887862000	4.174902000	29.081230000	XXXX	1	xx	Pd 0.000
Pd69	7.873338000	0.002444000	27.638973000	XXXX	1	xx	Pd 0.000
Pd70	1.971444000	4.177725000	26.218848000	XXXX	1	xx	Pd 0.000
Pd71	1.971282000	6.958313000	26.220221000	XXXX	1	xx	Pd 0.000
Pd72	1.968444000	1.391294000	26.215471000	XXXX	1	xx	Pd 0.000
Pd73	3.943801000	8.354151000	30.448469000	XXXX	1	xx	Pd 0.000
Pd74	1.861422000	1.390968000	29.109666000	XXXX	1	xx	Pd 0.000
Pd75	3.945957000	2.776425000	30.445038000	XXXX	1	xx	Pd 0.000
Pd76	5.906386000	6.957599000	26.223820000	XXXX	1	xx	Pd 0.000
Pd77	5.915040000	1.391415000	26.214696000	XXXX	1	xx	Pd 0.000

Pd78	5.906004000	4.178044000	26.222978000	XXXX 1	xx	Pd	0.000
N79	2.943769000	5.520875000	32.434981000	XXXX 1	xx	N	0.000
H80	5.111231000	6.981639000	30.649265000	XXXX 1	xx	H	0.000
H81	2.185924000	4.828379000	32.459442000	XXXX 1	xx	H	0.000
H82	5.114284000	4.148731000	30.643573000	XXXX 1	xx	H	0.000
H83	2.552733000	6.440795000	32.672359000	XXXX 1	xx	H	0.000
H84	3.645463000	5.267452000	33.139739000	XXXX 1	xx	H	0.000
H85	2.752595000	1.390707000	30.676628000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH_3/Pd(110) ($r_i = 0.375$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)	
Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.940681000	-0.002803000	24.798001000	XXXX 1	xx	Pd	0.000
Pd56	3.940628000	2.787012000	24.797325000	XXXX 1	xx	Pd	0.000

Pd57	3.937448000	5.568417000	24.803061000	XXXX 1	xx	Pd	0.000
Pd58	2.083041000	1.392103000	29.085849000	XXXX 1	xx	Pd	0.000
Pd59	2.084261000	4.173355000	29.107602000	XXXX 1	xx	Pd	0.000
Pd60	2.083627000	6.963116000	29.111180000	XXXX 1	xx	Pd	0.000
Pd61	7.883358000	0.007180000	30.499008000	XXXX 1	xx	Pd	0.000
Pd62	7.883365000	2.777059000	30.494496000	XXXX 1	xx	Pd	0.000
Pd63	7.880071000	5.567545000	30.657295000	XXXX 1	xx	Pd	0.000
Pd64	5.794232000	1.392531000	29.091218000	XXXX 1	xx	Pd	0.000
Pd65	5.797972000	4.168266000	29.109017000	XXXX 1	xx	Pd	0.000
Pd66	5.799434000	6.969635000	29.112971000	XXXX 1	xx	Pd	0.000
Pd67	7.877311000	0.001326000	27.670237000	XXXX 1	xx	Pd	0.000
Pd68	7.877011000	2.784571000	27.667884000	XXXX 1	xx	Pd	0.000
Pd69	7.877719000	5.568928000	27.759167000	XXXX 1	xx	Pd	0.000
Pd70	1.942830000	1.392531000	26.201827000	XXXX 1	xx	Pd	0.000
Pd71	1.929825000	4.180226000	26.219417000	XXXX 1	xx	Pd	0.000
Pd72	1.929578000	6.957323000	26.220727000	XXXX 1	xx	Pd	0.000
Pd73	3.933806000	8.352149000	27.616197000	XXXX 1	xx	Pd	0.000
Pd74	3.933771000	2.784583000	27.614524000	XXXX 1	xx	Pd	0.000
Pd75	3.926580000	5.569269000	27.627409000	XXXX 1	xx	Pd	0.000
Pd76	5.933904000	1.392182000	26.210551000	XXXX 1	xx	Pd	0.000
Pd77	5.941154000	4.181998000	26.225999000	XXXX 1	xx	Pd	0.000
Pd78	5.941451000	6.954964000	26.227695000	XXXX 1	xx	Pd	0.000
N79	-0.078514000	-2.818185000	32.901313000	XXXX 1	xx	N	0.000
H80	1.216257000	4.152853000	30.653804000	XXXX 1	xx	H	0.000
H81	8.725506000	5.362769000	33.298453000	XXXX 1	xx	H	0.000
H82	6.676532000	6.993154000	30.661912000	XXXX 1	xx	H	0.000
H83	6.667007000	1.392988000	30.661008000	XXXX 1	xx	H	0.000
H84	7.167194000	4.789043000	33.218297000	XXXX 1	xx	H	0.000
H85	-0.426858000	6.426006000	33.263770000	XXXX 1	xx	H	0.000
H86	1.215798000	6.983715000	30.661218000	XXXX 1	xx	H	0.000
H87	6.676241000	4.142850000	30.652302000	XXXX 1	xx	H	0.000
H88	1.227242000	1.393145000	30.662176000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH_3/Pd(110) ($r_i = 0.5$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd6	1.968585000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX 1	xx	Pd	0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX 1	xx	Pd	0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX 1	xx	Pd	0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX 1	xx	Pd	0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX 1	xx	Pd	0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX 1	xx	Pd	0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX 1	xx	Pd	0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX 1	xx	Pd	0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX 1	xx	Pd	0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX 1	xx	Pd	0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX 1	xx	Pd	0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX 1	xx	Pd	0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX 1	xx	Pd	0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX 1	xx	Pd	0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX 1	xx	Pd	0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX 1	xx	Pd	0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX 1	xx	Pd	0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX 1	xx	Pd	0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX 1	xx	Pd	0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX 1	xx	Pd	0.000

Pd33	5.921505000	6.960139000	17.831178000	XXXX 1	xx	Pd	0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX 1	xx	Pd	0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX 1	xx	Pd	0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX 1	xx	Pd	0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX 1	xx	Pd	0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX 1	xx	Pd	0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX 1	xx	Pd	0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX 1	xx	Pd	0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX 1	xx	Pd	0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX 1	xx	Pd	0.000
H43	4.784448000	2.783509000	14.813653000	XXXX 1	xx	H	0.000
H44	4.784327000	5.567528000	14.813308000	XXXX 1	xx	H	0.000
H45	4.784472000	8.351801000	14.814017000	XXXX 1	xx	H	0.000
H46	1.083094000	1.397647000	16.146732000	XXXX 1	xx	H	0.000
H47	1.082973000	4.181726000	16.146330000	XXXX 1	xx	H	0.000
H48	1.082856000	6.965576000	16.146515000	XXXX 1	xx	H	0.000
H49	2.883673000	1.392031000	16.147297000	XXXX 1	xx	H	0.000
H50	2.883493000	4.175967000	16.146767000	XXXX 1	xx	H	0.000
H51	2.883790000	6.960290000	16.147130000	XXXX 1	xx	H	0.000
H52	7.056651000	8.350437000	14.813892000	XXXX 1	xx	H	0.000
H53	7.056827000	2.782554000	14.813815000	XXXX 1	xx	H	0.000
H54	7.056528000	5.566429000	14.813346000	XXXX 1	xx	H	0.000
Pd55	3.936344000	0.001619000	24.795915000	XXXX 1	xx	Pd	0.000
Pd56	3.943977000	2.783661000	24.801796000	XXXX 1	xx	Pd	0.000
Pd57	3.937328000	5.566396000	24.796095000	XXXX 1	xx	Pd	0.000
Pd58	2.062194000	6.957474000	29.100426000	XXXX 1	xx	Pd	0.000
Pd59	2.053214000	1.368092000	29.113929000	XXXX 1	xx	Pd	0.000
Pd60	2.054382000	4.194818000	29.110215000	XXXX 1	xx	Pd	0.000
Pd61	0.014440000	-0.009039000	30.551058000	XXXX 1	xx	Pd	0.000
Pd62	0.020992000	2.781763000	30.685087000	XXXX 1	xx	Pd	0.000
Pd63	0.013835000	5.570069000	30.545591000	XXXX 1	xx	Pd	0.000
Pd64	5.831795000	1.404522000	29.139331000	XXXX 1	xx	Pd	0.000
Pd65	5.830876000	4.157536000	29.137006000	XXXX 1	xx	Pd	0.000
Pd66	5.833597000	6.957358000	29.132097000	XXXX 1	xx	Pd	0.000
Pd67	7.874457000	0.000058000	27.681584000	XXXX 1	xx	Pd	0.000
Pd68	7.882691000	2.782378000	27.749224000	XXXX 1	xx	Pd	0.000
Pd69	7.873240000	5.566759000	27.678558000	XXXX 1	xx	Pd	0.000
Pd70	1.935950000	1.398532000	26.211412000	XXXX 1	xx	Pd	0.000
Pd71	1.935936000	4.167514000	26.210259000	XXXX 1	xx	Pd	0.000
Pd72	1.930014000	6.959307000	26.206874000	XXXX 1	xx	Pd	0.000
Pd73	3.918692000	-0.002005000	27.600296000	XXXX 1	xx	Pd	0.000
Pd74	3.963484000	2.781984000	27.612275000	XXXX 1	xx	Pd	0.000
Pd75	3.919843000	5.567550000	27.598210000	XXXX 1	xx	Pd	0.000
Pd76	5.949083000	1.393279000	26.223773000	XXXX 1	xx	Pd	0.000
Pd77	5.948740000	4.176647000	26.222788000	XXXX 1	xx	Pd	0.000
Pd78	5.933044000	6.963738000	26.202250000	XXXX 1	xx	Pd	0.000
N79	0.249247000	2.815329000	32.918031000	XXXX 1	xx	N	0.000
H80	3.191881000	2.779821000	29.233383000	XXXX 1	xx	H	0.000
H81	1.218873000	6.955161000	30.693104000	XXXX 1	xx	H	0.000
H82	6.690377000	4.192437000	30.704824000	XXXX 1	xx	H	0.000
H83	0.727104000	3.672417000	33.217586000	XXXX 1	xx	H	0.000
H84	4.665513000	5.542576000	29.227033000	XXXX 1	xx	H	0.000
H85	4.665771000	0.018458000	29.228578000	XXXX 1	xx	H	0.000
H86	0.801022000	2.012299000	33.233909000	XXXX 1	xx	H	0.000
H87	-0.667581000	2.780172000	33.374612000	XXXX 1	xx	H	0.000
H88	1.212064000	4.196881000	30.668055000	XXXX 1	xx	H	0.000
H89	6.700571000	6.956018000	30.727618000	XXXX 1	xx	H	0.000
H90	1.210722000	1.363215000	30.675732000	XXXX 1	xx	H	0.000
H91	6.691852000	1.366360000	30.708915000	XXXX 1	xx	H	0.000

end

H_{r_i}-NH_3/Pd(110) ($r_i = 1$)

PBC	7.8743	8.3520	45.3120	90.0000	90.0000	90.0000 (P1)

Pd1	5.905756000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd2	5.905756000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000
Pd3	5.905756000	6.959972000	23.351992000	XXXX 1	xx	Pd	0.000
Pd4	1.968585000	1.392028000	23.351992000	XXXX 1	xx	Pd	0.000
Pd5	1.968585000	4.176000000	23.351992000	XXXX 1	xx	Pd	0.000

Pd6	1.968585000	6.959972000	23.351992000	XXXX	1	xx	Pd 0.000
Pd7	0.000000000	2.783972000	24.743977000	XXXX	1	xx	Pd 0.000
Pd8	0.000000000	5.568028000	24.743977000	XXXX	1	xx	Pd 0.000
Pd9	0.000000000	0.000000000	24.743977000	XXXX	1	xx	Pd 0.000
Pd10	0.000000000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd11	0.000000000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd12	0.000000000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd13	1.968585000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd14	1.968585000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd15	1.968585000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd16	3.937171000	0.000000000	21.960008000	XXXX	1	xx	Pd 0.000
Pd17	3.937171000	2.783972000	21.960008000	XXXX	1	xx	Pd 0.000
Pd18	3.937171000	5.568028000	21.960008000	XXXX	1	xx	Pd 0.000
Pd19	5.905756000	1.392028000	20.568023000	XXXX	1	xx	Pd 0.000
Pd20	5.905756000	4.176000000	20.568023000	XXXX	1	xx	Pd 0.000
Pd21	5.905756000	6.959972000	20.568023000	XXXX	1	xx	Pd 0.000
Pd22	3.937171000	0.000000000	19.176038000	XXXX	1	xx	Pd 0.000
Pd23	3.937171000	2.783972000	19.176038000	XXXX	1	xx	Pd 0.000
Pd24	3.937171000	5.568028000	19.176038000	XXXX	1	xx	Pd 0.000
Pd25	0.030552000	0.000585000	19.175585000	XXXX	1	xx	Pd 0.000
Pd26	0.030552000	2.784640000	19.175585000	XXXX	1	xx	Pd 0.000
Pd27	0.030474000	5.568612000	19.175585000	XXXX	1	xx	Pd 0.000
Pd28	1.984491000	1.391777000	17.725601000	XXXX	1	xx	Pd 0.000
Pd29	1.984413000	4.175749000	17.725148000	XXXX	1	xx	Pd 0.000
Pd30	1.984334000	6.959638000	17.725148000	XXXX	1	xx	Pd 0.000
Pd31	5.921662000	1.392362000	17.831631000	XXXX	1	xx	Pd 0.000
Pd32	5.921426000	4.176251000	17.831178000	XXXX	1	xx	Pd 0.000
Pd33	5.921505000	6.960139000	17.831178000	XXXX	1	xx	Pd 0.000
Pd34	0.040002000	8.351749000	16.401585000	XXXX	1	xx	Pd 0.000
Pd35	0.040159000	2.783638000	16.401585000	XXXX	1	xx	Pd 0.000
Pd36	0.039844000	5.567527000	16.401132000	XXXX	1	xx	Pd 0.000
Pd37	3.928115000	2.783388000	16.402491000	XXXX	1	xx	Pd 0.000
Pd38	3.928036000	5.567193000	16.402038000	XXXX	1	xx	Pd 0.000
Pd39	3.928351000	8.351499000	16.402944000	XXXX	1	xx	Pd 0.000
Pd40	5.920323000	1.391026000	15.136474000	XXXX	1	xx	Pd 0.000
Pd41	5.920087000	4.174831000	15.136020000	XXXX	1	xx	Pd 0.000
Pd42	5.920008000	6.958803000	15.136020000	XXXX	1	xx	Pd 0.000
H43	4.784448000	2.783509000	14.813653000	XXXX	1	xx	H 0.000
H44	4.784327000	5.567528000	14.813308000	XXXX	1	xx	H 0.000
H45	4.784472000	8.351801000	14.814017000	XXXX	1	xx	H 0.000
H46	1.083094000	1.397647000	16.146732000	XXXX	1	xx	H 0.000
H47	1.082973000	4.181726000	16.146330000	XXXX	1	xx	H 0.000
H48	1.082856000	6.965576000	16.146515000	XXXX	1	xx	H 0.000
H49	2.883673000	1.392031000	16.147297000	XXXX	1	xx	H 0.000
H50	2.883493000	4.175967000	16.146767000	XXXX	1	xx	H 0.000
H51	2.883790000	6.960290000	16.147130000	XXXX	1	xx	H 0.000
H52	7.056651000	8.350437000	14.813892000	XXXX	1	xx	H 0.000
H53	7.056827000	2.782554000	14.813815000	XXXX	1	xx	H 0.000
H54	7.056528000	5.566429000	14.813346000	XXXX	1	xx	H 0.000
Pd55	3.935535000	8.347911000	24.821098000	XXXX	1	xx	Pd 0.000
Pd56	3.935219000	2.784332000	24.817667000	XXXX	1	xx	Pd 0.000
Pd57	3.934349000	5.566300000	24.830912000	XXXX	1	xx	Pd 0.000
Pd58	3.994503000	2.779830000	28.214248000	XXXX	1	xx	Pd 0.000
Pd59	6.234498000	1.386958000	29.700603000	XXXX	1	xx	Pd 0.000
Pd60	3.964619000	5.557068000	31.171607000	XXXX	1	xx	Pd 0.000
Pd61	1.838599000	1.385522000	29.630961000	XXXX	1	xx	Pd 0.000
Pd62	1.839352000	6.959429000	29.635297000	XXXX	1	xx	Pd 0.000
Pd63	3.997922000	2.768775000	31.002050000	XXXX	1	xx	Pd 0.000
Pd64	3.996197000	8.346229000	31.008906000	XXXX	1	xx	Pd 0.000
Pd65	1.839318000	4.163703000	29.625117000	XXXX	1	xx	Pd 0.000
Pd66	6.228693000	6.957709000	29.721993000	XXXX	1	xx	Pd 0.000
Pd67	0.004335000	8.348301000	27.941489000	XXXX	1	xx	Pd 0.000
Pd68	0.003844000	2.780281000	27.940262000	XXXX	1	xx	Pd 0.000
Pd69	0.002025000	5.565132000	27.955609000	XXXX	1	xx	Pd 0.000
Pd70	2.032226000	1.389336000	26.567872000	XXXX	1	xx	Pd 0.000
Pd71	2.040597000	4.179699000	26.582238000	XXXX	1	xx	Pd 0.000
Pd72	2.040351000	6.951258000	26.584515000	XXXX	1	xx	Pd 0.000
Pd73	3.990776000	5.564790000	28.325573000	XXXX	1	xx	Pd 0.000
Pd74	3.994262000	8.348657000	28.219315000	XXXX	1	xx	Pd 0.000

Pd75	6.229502000	4.170825000	29.719288000	XXXX 1	xx	Pd 0.000
Pd76	5.806989000	1.388868000	26.370565000	XXXX 1	xx	Pd 0.000
Pd77	5.796139000	4.178488000	26.391739000	XXXX 1	xx	Pd 0.000
Pd78	5.796079000	6.953857000	26.396604000	XXXX 1	xx	Pd 0.000
H79	5.262566000	6.945105000	28.197726000	XXXX 1	xx	H 0.000
H80	2.793772000	4.118241000	31.155158000	XXXX 1	xx	H 0.000
H81	5.269386000	1.387552000	28.160403000	XXXX 1	xx	H 0.000
H82	5.261201000	4.183007000	28.197215000	XXXX 1	xx	H 0.000
H83	1.228534000	6.959379000	24.987046000	XXXX 1	xx	H 0.000
H84	6.986343000	2.787643000	26.329715000	XXXX 1	xx	H 0.000
H85	5.163991000	4.165689000	31.173158000	XXXX 1	xx	H 0.000
H86	6.986768000	8.339602000	26.329421000	XXXX 1	xx	H 0.000
H87	0.645249000	8.345313000	29.653208000	XXXX 1	xx	H 0.000
H88	3.311930000	5.564767000	26.551430000	XXXX 1	xx	H 0.000
H89	3.297810000	2.779308000	26.521896000	XXXX 1	xx	H 0.000
H90	3.297413000	8.348927000	26.527264000	XXXX 1	xx	H 0.000
H91	1.216486000	1.392409000	24.977149000	XXXX 1	xx	H 0.000
H92	2.792206000	6.991790000	31.173719000	XXXX 1	xx	H 0.000
H93	5.163048000	6.948574000	31.179420000	XXXX 1	xx	H 0.000
H94	0.670097000	5.562571000	29.663784000	XXXX 1	xx	H 0.000
H95	0.645880000	2.775744000	29.653791000	XXXX 1	xx	H 0.000
H96	1.227895000	4.176820000	24.986058000	XXXX 1	xx	H 0.000
H97	3.683972000	6.461179000	33.830923000	XXXX 1	xx	H 0.000
H98	6.990934000	5.563687000	26.334247000	XXXX 1	xx	H 0.000
H99	4.425297000	4.976521000	33.908117000	XXXX 1	xx	H 0.000
H100	2.817263000	1.381919000	31.185643000	XXXX 1	xx	H 0.000
H101	5.189616000	1.379650000	31.177678000	XXXX 1	xx	H 0.000
H102	2.789247000	5.077080000	33.647406000	XXXX 1	xx	H 0.000
N103	3.692799000	5.516441000	33.437499000	XXXX 1	xx	N 0.000

end