

Supporting Information

for

Identifying non-proton-coupled electron transfer as a potential limiting step for the electrosynthesis of ammonia

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Methodology

Quantum calculations. Spin-polarized density function theory (DFT)^{1, 2} calculations were performed using the DMol³ package. A generalized gradient approximation (GGA)^{3, 4} in the form of revised-Perdew-Burke-Ernzerhof (RPBE) functional⁵ was utilized to account for the exchange-correlation interaction, accompanied by the DFT-D2⁶ semi-empirical method to estimate the dispersion correction. The DFT semi-core pseudopotential (DSPP) method⁷ for the numeric atomic orbital basis set was implemented to treat the core electron interactions. A Γ -centered k-point grid of $4 \times 4 \times 1$ was employed to sample the Brillouin zone in structural relaxation, while an $8 \times 8 \times 1$ k-point mesh was used for electronic properties calculations. The convergence tolerances of energy, force, and displacement for geometry optimization were set as 1.0×10^{-6} Ha, 1.0×10^{-3} Ha/Å, and 5.0×10^{-3} Å, respectively. The Gaussian smearing with a smearing width of 5.0×10^{-3} Ha was used to accelerate the convergence. The distance of vacuum layer in the z-direction was set to 20 Å to eliminate the interactions between periodic regions. Ab initio molecular dynamics (AIMD) simulations with NVT ensemble were conducted to evaluate the dynamic stability.

The minimum energy paths (MEP) were determined by the linear synchronous transit/quadratic synchronous transit (LST/QST) methods⁸ with a root mean squared (RMS) convergence of 1.0×10^{-3} Ha/Å and further confirmed by the nudged elastic band (NEB) method⁹. The reaction Gibbs free energy change (ΔG) of the elementary steps was constructed based on the computational hydrogen electrode (CHE) theory developed by Nørskov et al.¹⁰, where the chemical potential of ($H^+ + e^-$) pair in solution was equal to the half of the chemical potential of a gas-phase H_2 and the reference potential was set to reversible hydrogen electrode (RHE). The corresponding ΔG can be calculated by

$$\Delta G = \Delta E + \Delta ZPE - T\Delta S$$

where ΔE is the total DFT energy, ΔZPE and ΔS are the contributions of zero point energy and entropy to the ΔG . In this study, the temperature T is 298.15 K. The limiting potential (U_L) was defined as $U_L = -\Delta G_{\max}/e$, where ΔG_{\max} is the free energy change of potential limiting step (PLS).

Machine learning (ML). The ML scheme of homemade code was accomplished within Numpy¹¹, Pandas¹², Scikit-learn¹³, and XGBoost¹⁴ packages, as performed in the Python3 environment. Five state-of-the-art ML algorithms, namely, Support Vector Regression (SVR)¹⁵, Kernel ridge regression (KRR)¹⁶, Least Absolute Shrinkage and Selection Operator Regression (LASSO)¹⁷, Random Forest Regression (RFR)^{18, 19}, and eXtreme Gradient Boosting Regression (XGBoost)¹⁴ were employed to build the ML models. With the aid of the Optuna²⁰, the optimal hyper-parameters were successfully searched, as available in **Table S12**. Taking the XGBoost model as an example, the `n_estimators`, `max_depth`, `min_child_weight`, `learning_rate`, `colsample_bytree`, `subsample`, `reg_alpha`, `reg_lambda` and `gamma` were considered to seek the optimal hyper-parameters using Optuna algorithm.

After normalization pre-processing²¹, the raw data calculated by DFT were randomly shuffled and divided into train and test sets with the ratio of 4 : 1. To avoid the risk of over-fitting, 10-fold cross validation²² was executed in the process of training ML model. The values of the coefficients of determination (R^2) and root mean square error (RMSE) were utilized to estimate the errors of five algorithms, in which R^2 represents the proportion of variance that has been parsed by the independent variables in the corresponding model, while RMSE stands for the differences between the ML-predicted and DFT-calculated results. That is, a ML model endowed with better generalization ability corresponds to a smaller RMSE and larger R^2 . In addition, the SHapley

Additive exPlanation (SHAP)²³⁻²⁵ was adopted to elucidate the output of the ML models. Based on the optimal ML model, the algorithm of SHAP was used to calculate the importance of input features.

Based on the optimized adsorption configurations via DFT method, the many-body tensor representation (MBTR)²⁶ was adopted to encode the structure through the Dscribe 2.1.0²⁷. As given in **Table S13**, the parameters were used to perform the calculation of MBTR. Then, the principal component analysis (PCA) was used to decrease the dimensionality of the dataset generated by MBTR, reducing the dimensionality to 6 and combined these data with Z , X , N , N_d , I_1 and R_d as dataset for subsequent ML.

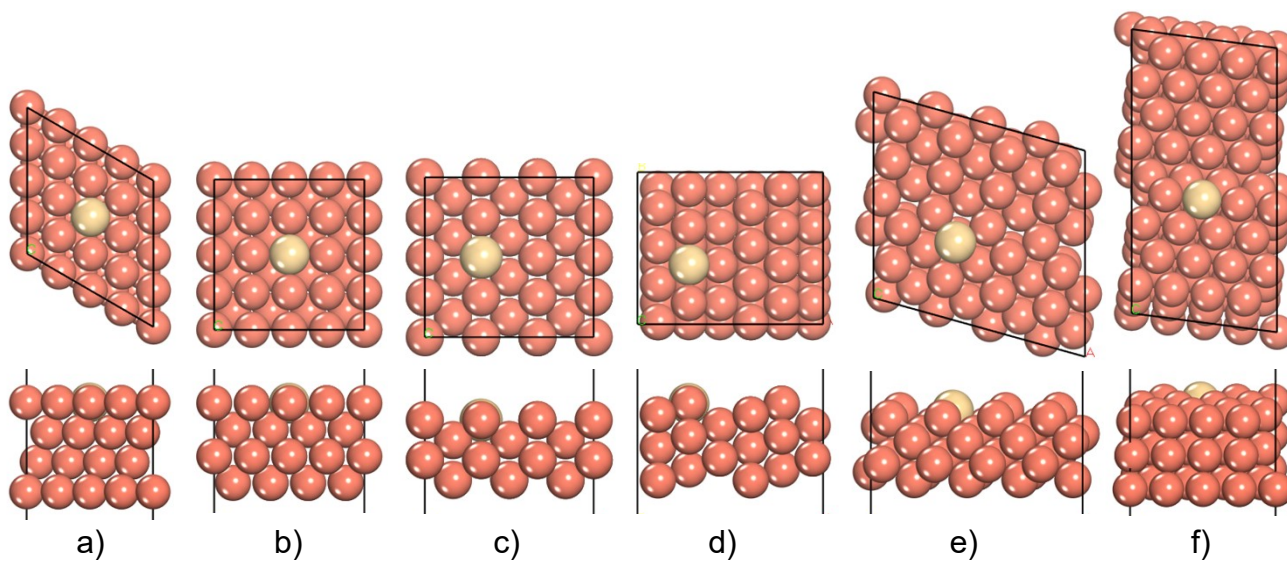


Figure S1. Top and side views of six optimized Cu-based configurations with different Miller index, denoted as (a) TM/Cu(111), (b) TM/Cu(100), (c) TM/Cu(110), (d) TM/Cu(211), (e) TM/Cu(320) and (f) TM/Cu(553) where the TM and Cu atoms are labeled by earthy yellow and pink, respectively.

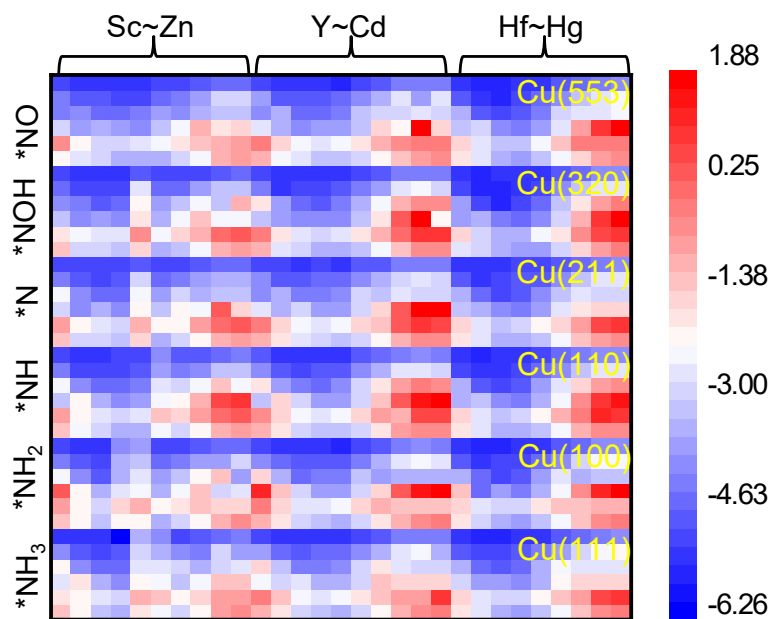


Figure S2. Hot spot map of adsorption free energy distribution of six different intermediates (*NO, *NOH, *N, *NH, *NH₂ and *NH₃).

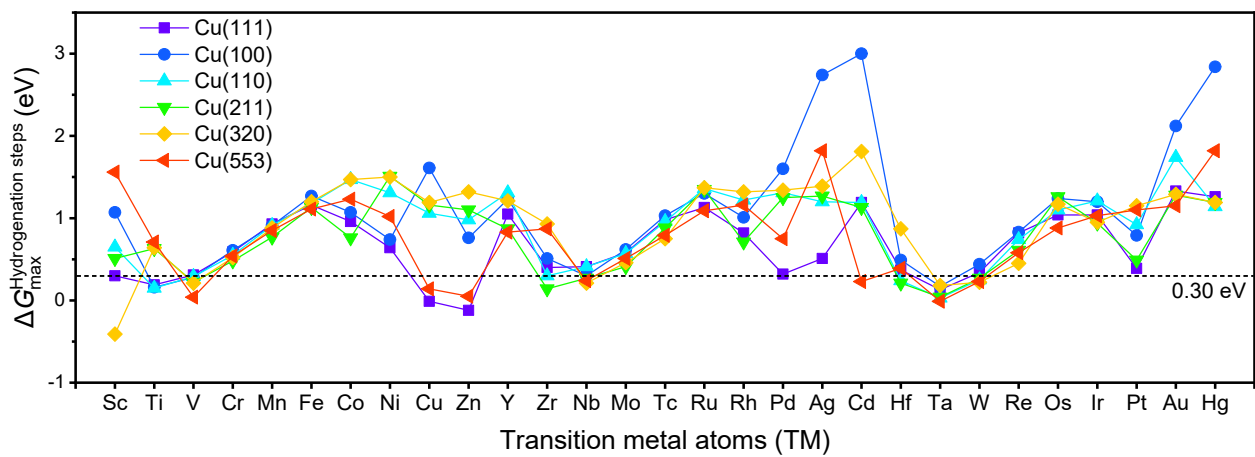


Figure S3. The maximum Gibbs free energy changes of all studied systems during hydrogenation steps.

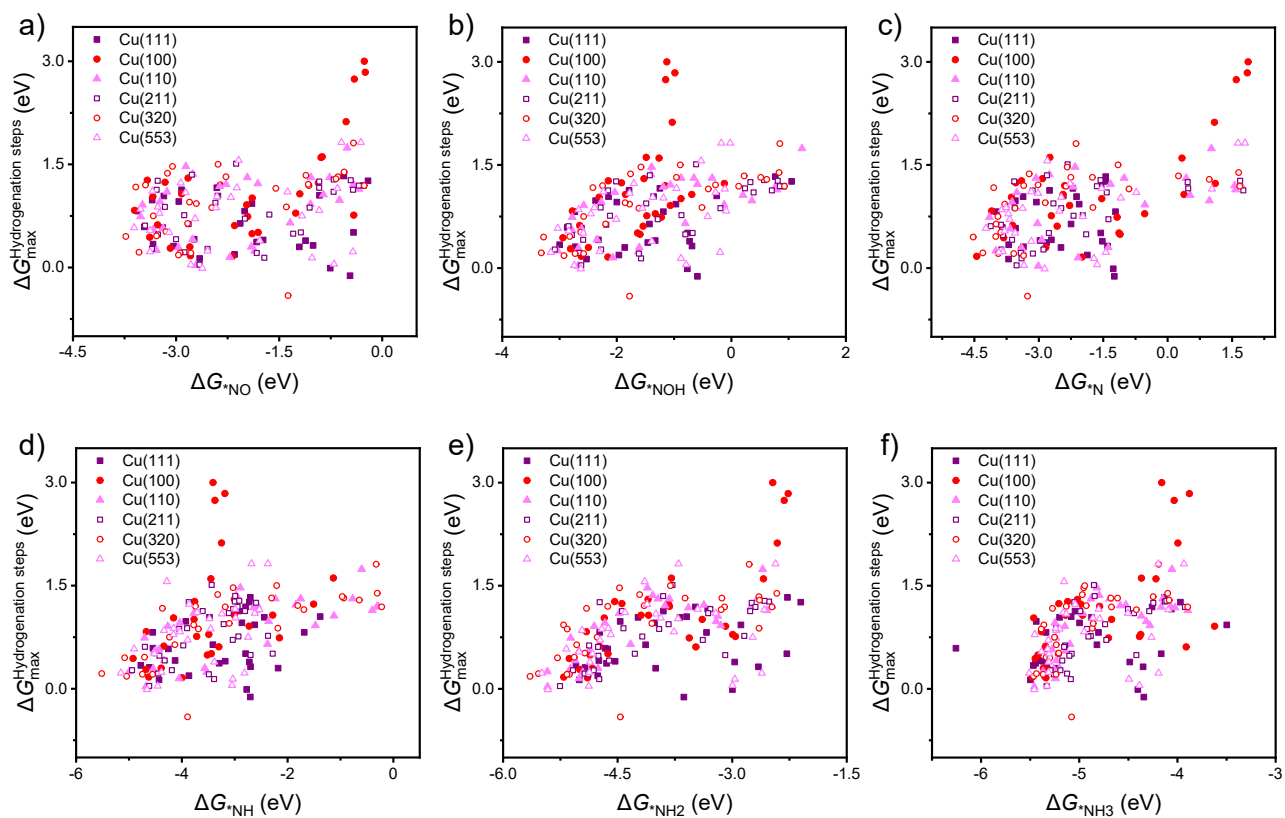


Figure S4. Scaling relationships of the adsorption Gibbs free energy changes of ΔG^*_{NO} (a), ΔG^*_{NOH} (b), ΔG^*_N (c), ΔG^*_{NH} (d), $\Delta G^*_{\text{NH}_2}$ (e), and $\Delta G^*_{\text{NH}_3}$ (f) as a function of the maximum Gibbs free energy changes of all studied systems during hydrogenation steps.

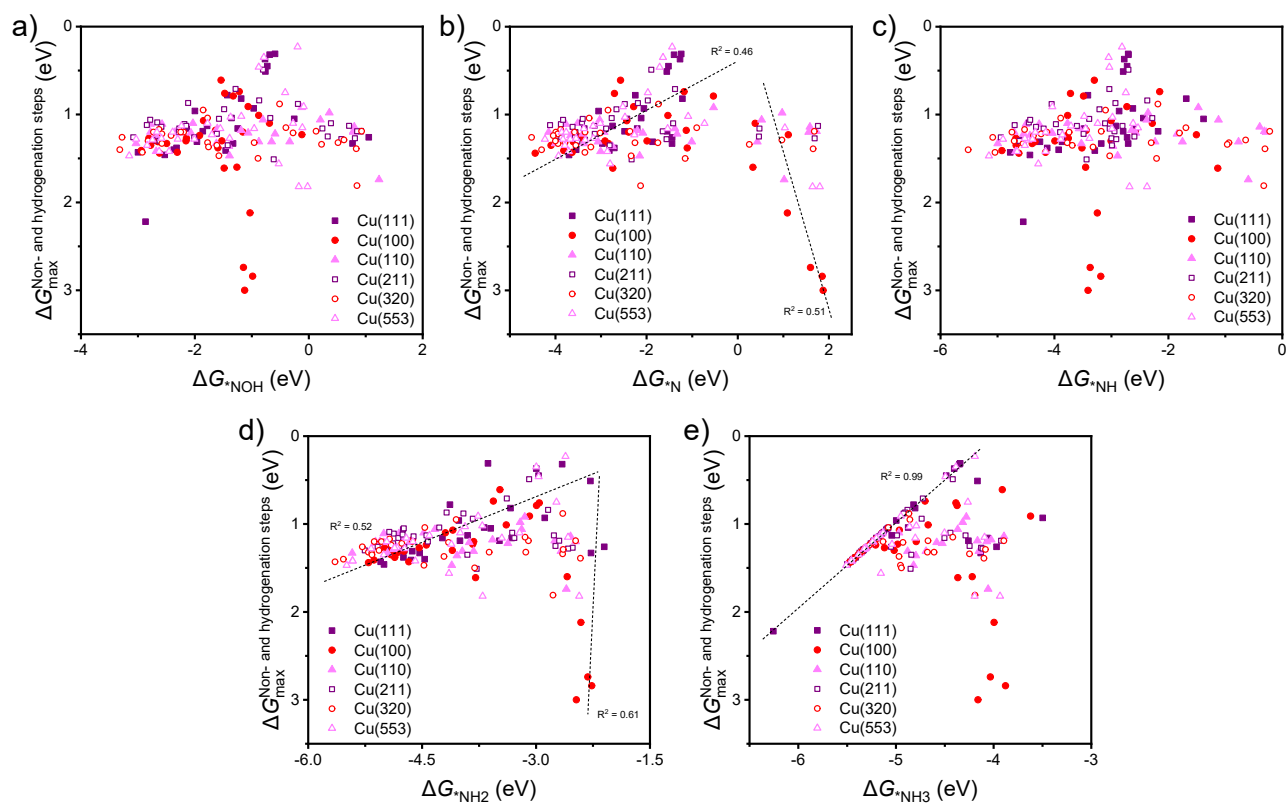


Figure S5. Scaling relationships of the adsorption Gibbs free energy changes of ΔG^*_{NOH} (a), ΔG^*_{N} (b), ΔG^*_{NH} (c), $\Delta G^*_{\text{NH}_2}$ (d), and $\Delta G^*_{\text{NH}_3}$ (e) as a function of the maximum Gibbs free energy changes of all studied systems during non- and hydrogenation steps.

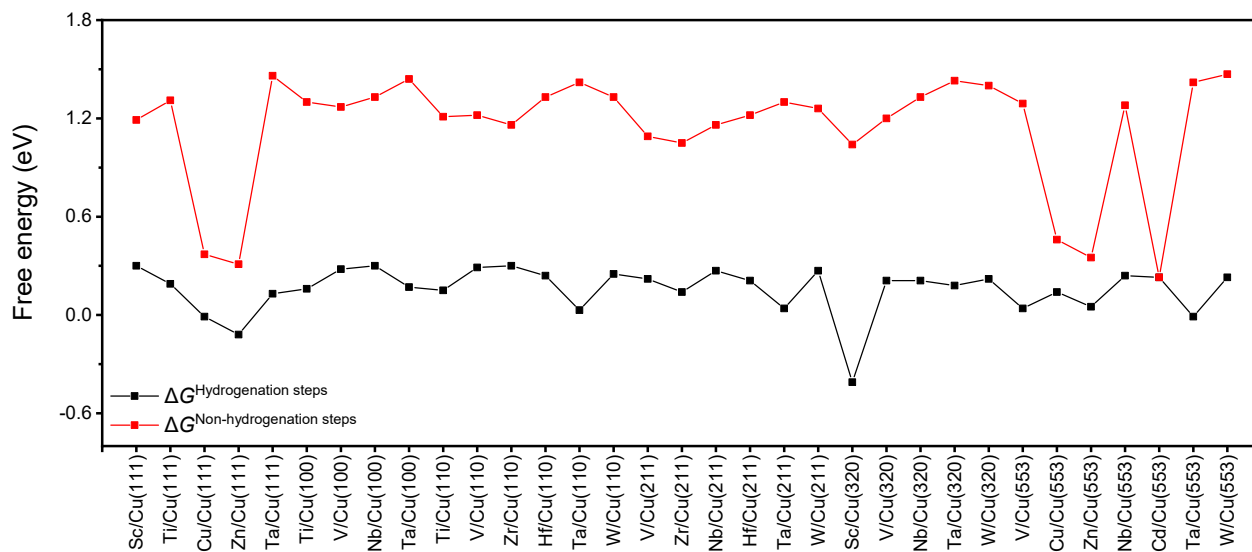


Figure S6. The difference in maximum Gibbs free energy changes of 33 screened catalysts when considering hydrogenation and non-hydrogenation steps.

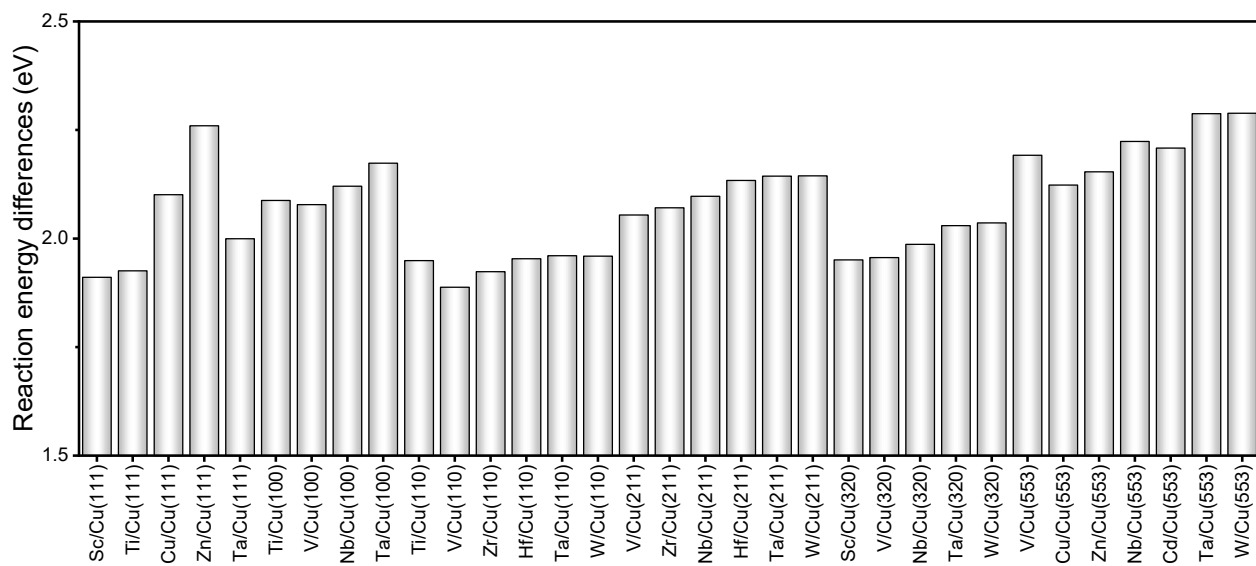


Figure S7. Reaction energy differences between $^*\text{NH}_3 + \text{H}_5\text{O}_2^+ \rightarrow ^* + \text{NH}_4^+ + 2\text{H}_2\text{O}$ and $^*\text{NH}_3 + \text{H}_5\text{O}_2^+ \rightarrow ^* + \text{NH}_3 + \text{H}_5\text{O}_2^+$ of 33 screened catalysts.

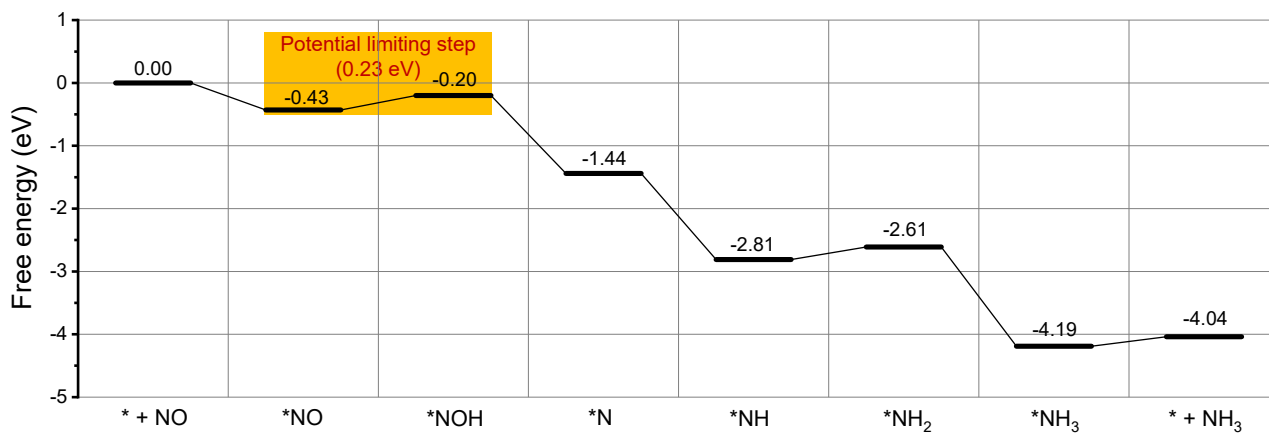


Figure S9. Gibbs free energy profile of O-distal mechanism on Cd/Cu(553) at $U = 0$ V.

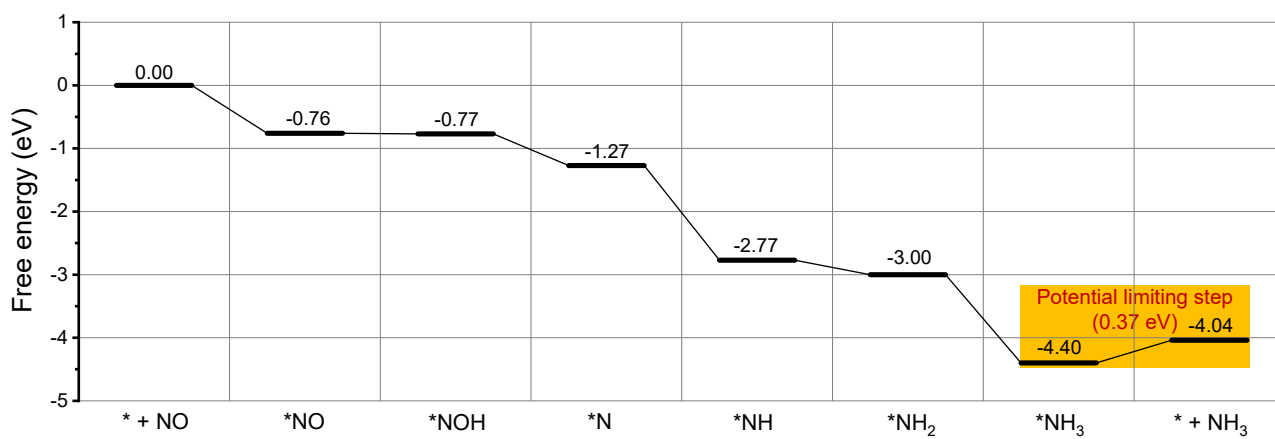


Figure S10. Gibbs free energy profile of O-distal mechanism on Cu/Cu(111) at $U = 0$ V.

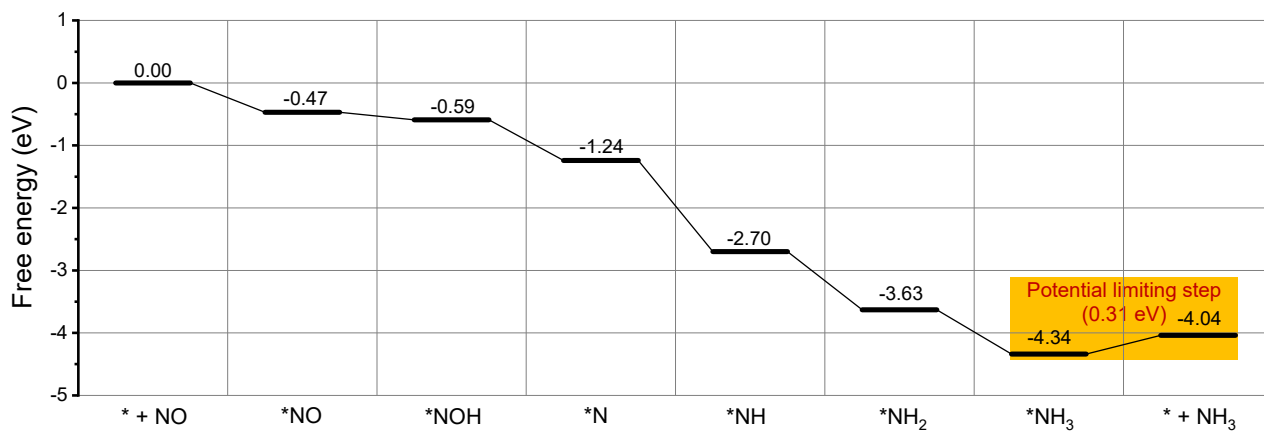


Figure S11. Gibbs free energy profile of O-distal mechanism on Zn/Cu(111) at $U = 0$ V.

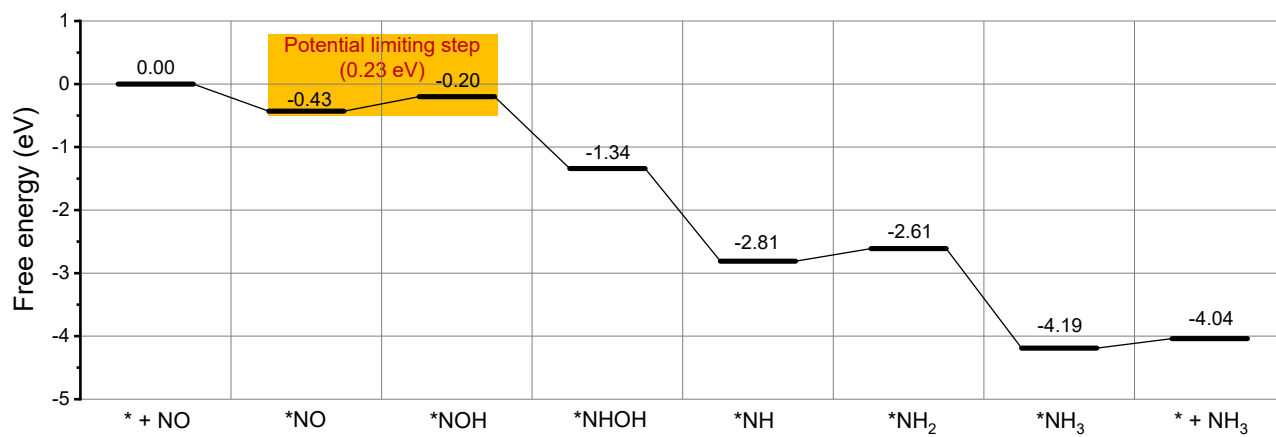


Figure S12. Gibbs free energy profile of O-alternative mechanism on Cd/Cu(553) at $U = 0$ V.

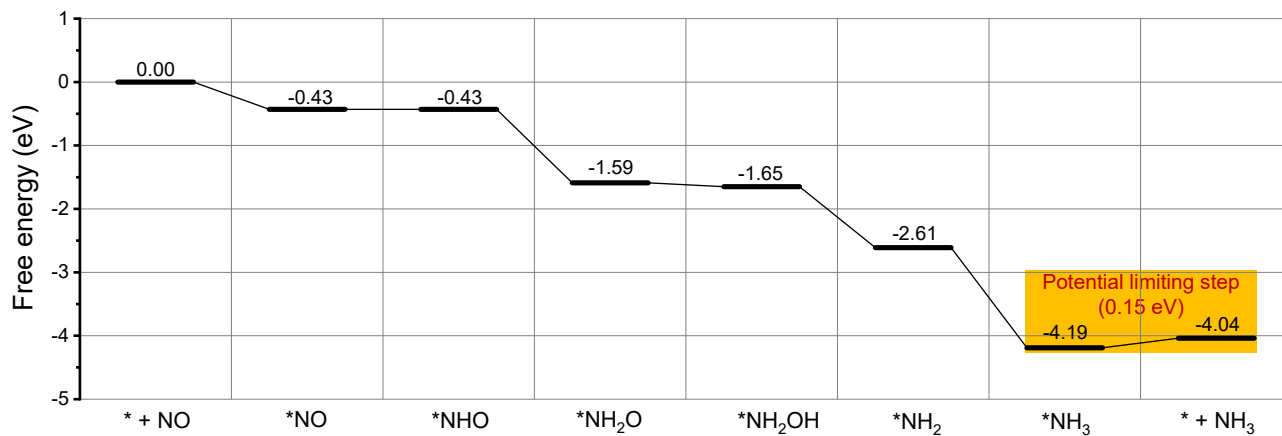


Figure S13. Gibbs free energy profile of N-distal mechanism on Cd/Cu(553) at $U = 0$ V.

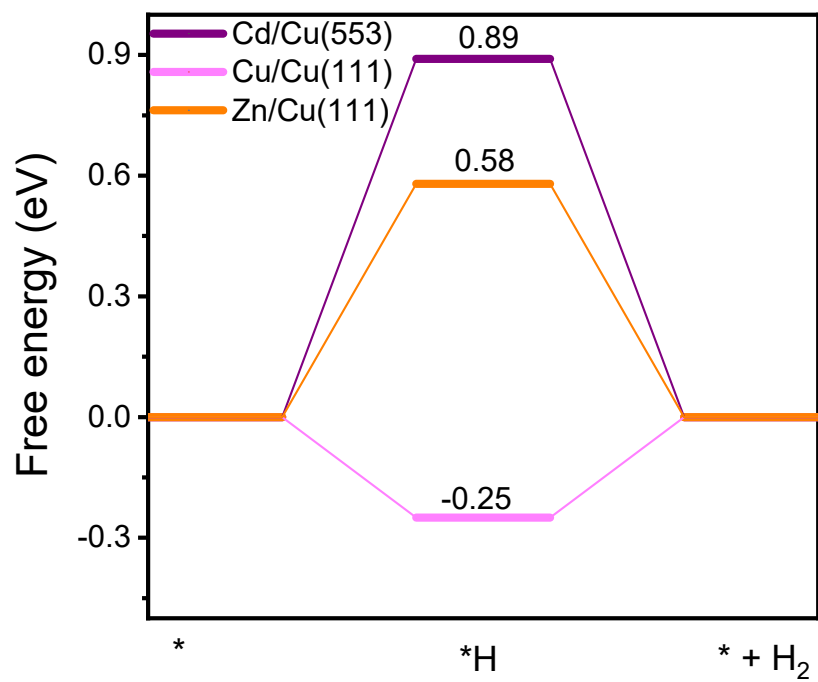


Figure S14. Gibbs free energy profile of HER at $U = 0$ V.

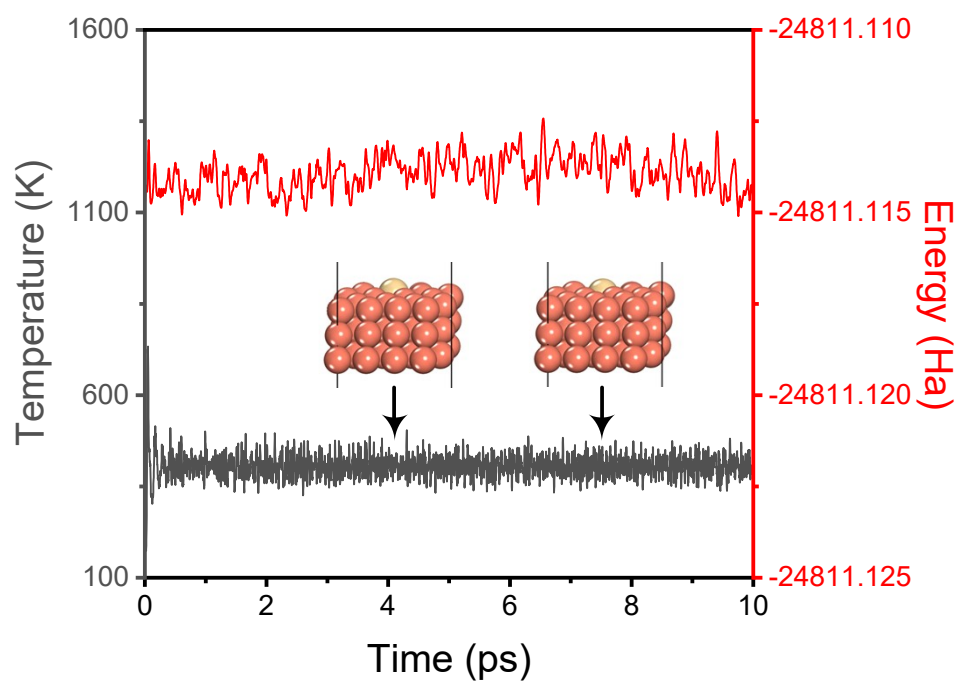


Figure S15. Temperature and total energy changes during AIMD simulations within 10 ps under 400 K for Cd/Cu(553), of which the snapshots at 4.0 and 7.5 ps are inset.

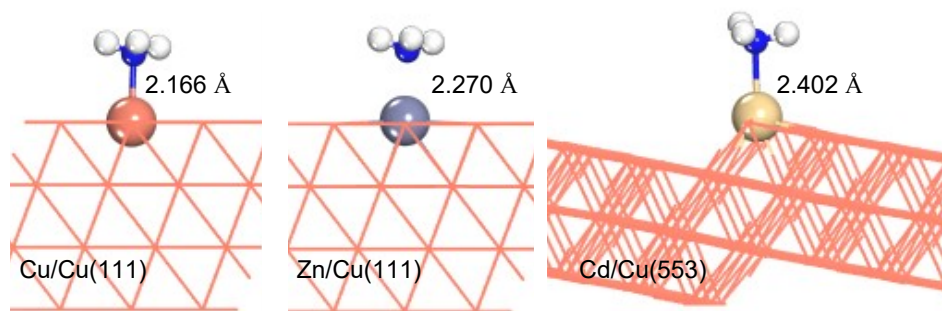


Figure S16. The optimized *NH₃ configurations of Cu/Cu(111), Zn/Cu(111) and Cd/Cu(553), where the bond lengths of TM-N are marked inset, respectively.

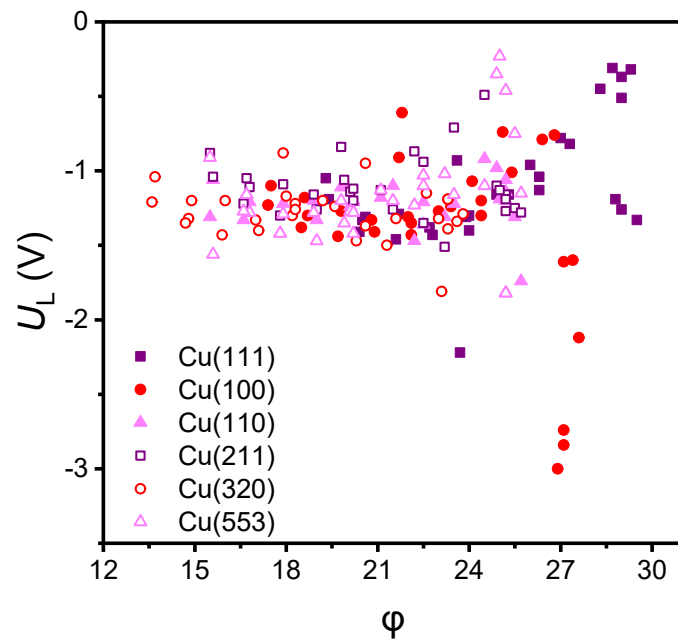


Figure S17. Scaling relationships of the descriptor ϕ (proposed by Wang et al.²⁸) as a function of the U_L .

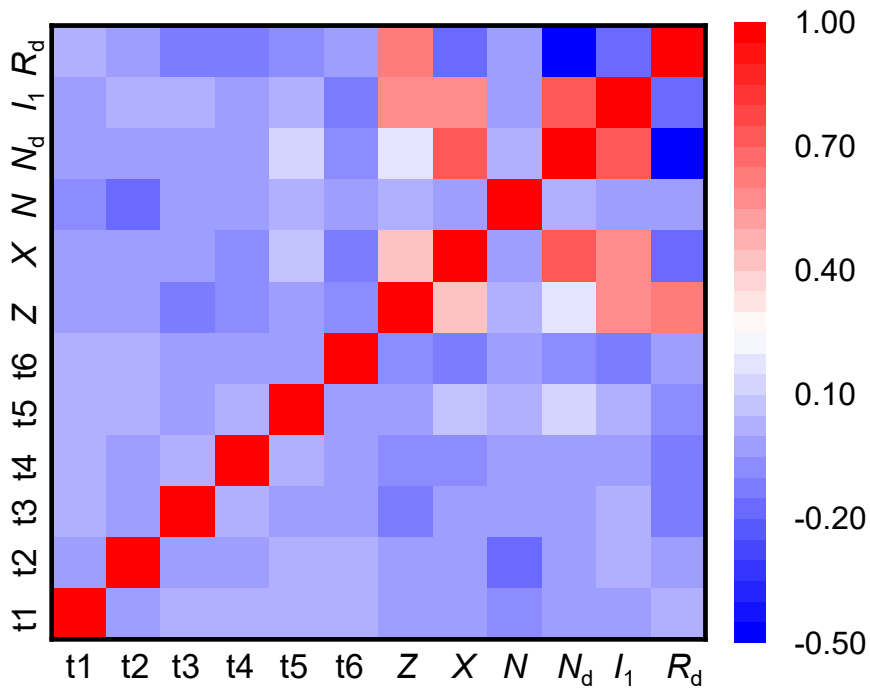


Figure S18. Pearson correlation coefficient matrix analysis for the 12 features selected for the ML analysis.

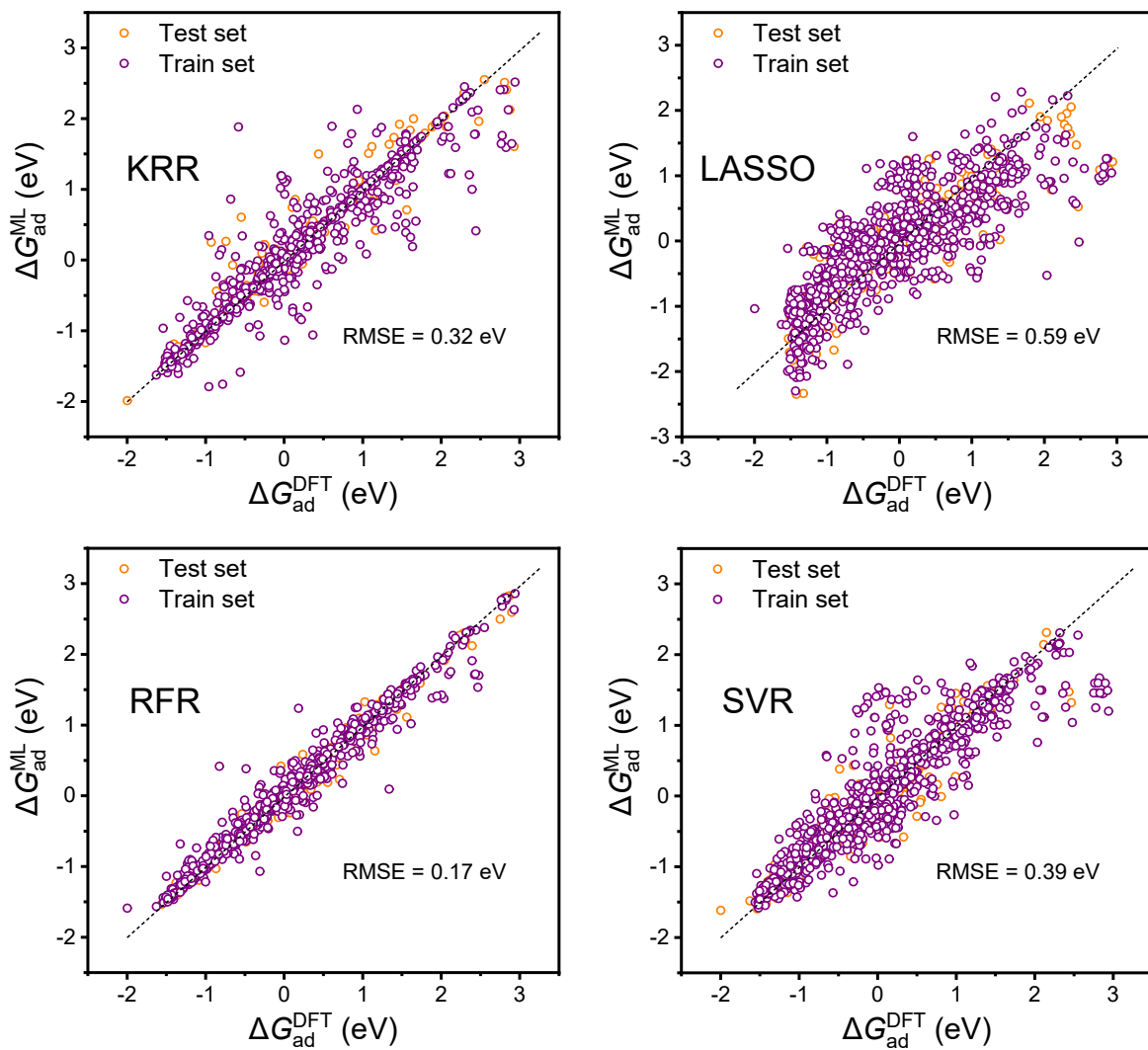


Figure S19. Comparison of DFT calculated ΔG_{ads} values with those predicted by ML methods.

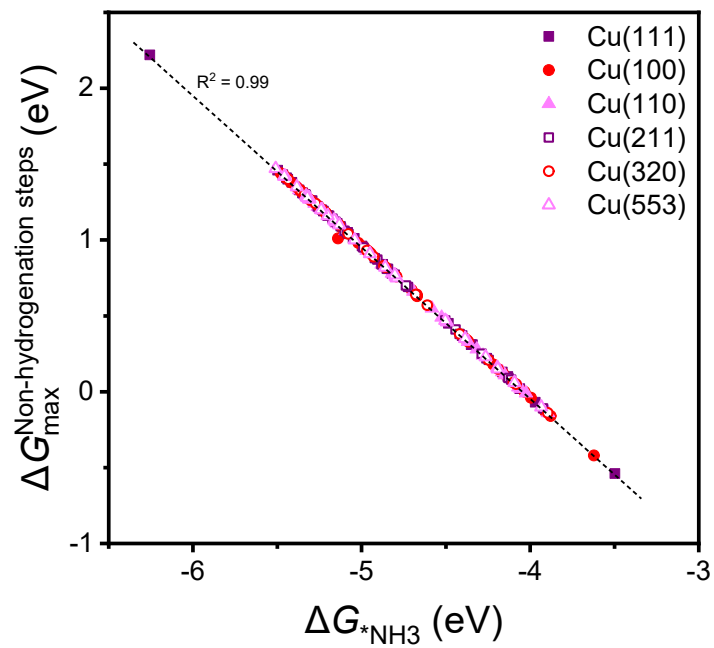


Figure S20. Scaling relationships of the adsorption Gibbs free energy changes of $\Delta G_{\text{NH}_3}^*$ as a function of the maximum Gibbs free energy changes of all studied systems during non-hydrogenation steps.

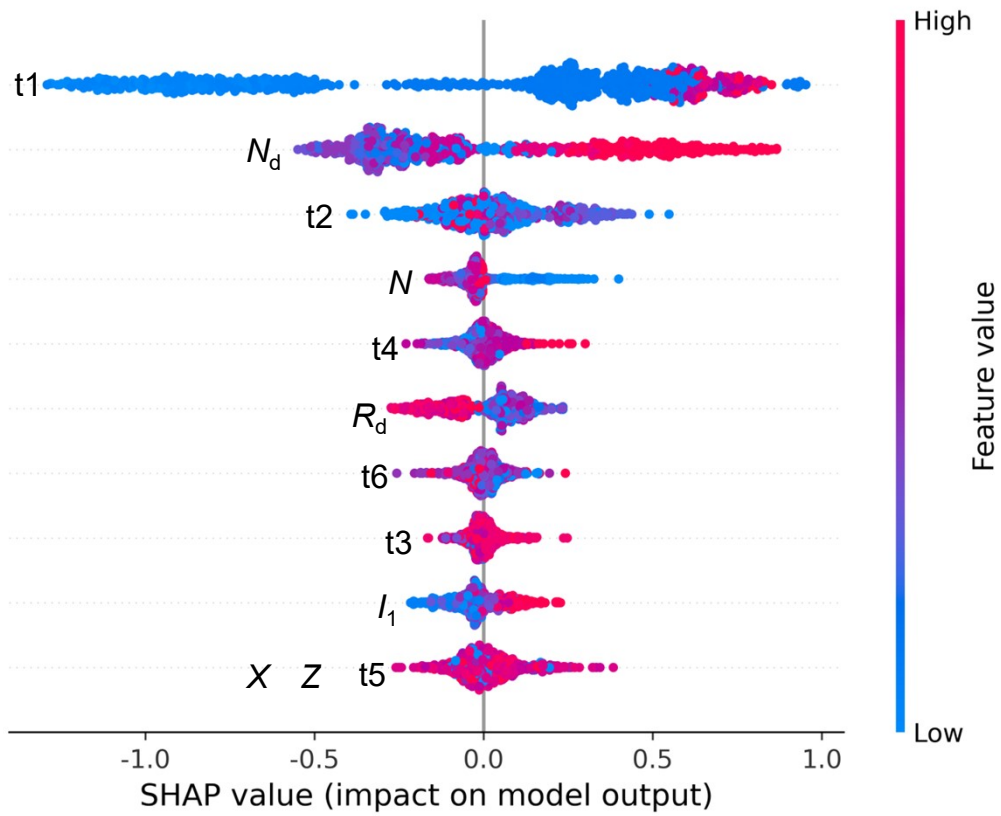


Figure S21. Beeswarm graph of each sample under the XGBoost model. The color scale corresponds to the feature values. Red and blue colors represent the large and small feature values, respectively.

Table S1. The lattice parameters of six optimized Cu-based structures with different Miller index.

	Cu(111)	Cu(100)	Cu(110)	Cu(211)	Cu(320)	Cu(553)
a (Å)	10.5172	10.5172	11.1552	12.8809	14.8736	10.5172
b (Å)	10.5172	10.5172	10.5172	10.5172	13.9130	20.3665
c (Å)	26.4405	25.5776	23.9440	25.3131	24.6408	26.2932

Table S2. Formation energies of all SAA catalysts (eV).

TM	Cu(111)	Cu(100)	Cu(110)	Cu(211)	Cu(320)	Cu(553)
Sc	-5.72	-5.29	-4.89	-3.91	-2.34	-1.47
Ti	-6.27	-5.84	-4.95	-4.44	-3.20	-3.72
V	-6.01	-5.53	-4.35	-4.13	-3.22	-4.46
Cr	-2.71	-3.69	-1.88	-0.83	0.95	1.27
Mn	-4.24	-3.86	-1.84	-2.54	-1.09	1.53
Fe	-4.33	-2.94	-3.42	-1.64	-0.29	-0.38
Co	-5.62	-5.18	-4.34	-3.97	-3.25	-4.11
Ni	-7.27	-6.79	-5.84	-5.55	-4.91	-5.67
Cu	-7.35	-6.82	-5.98	-5.85	-5.48	-5.93
Zn	-7.71	-7.12	-6.30	-6.22	-6.01	-6.35
Y	-8.13	-7.81	-6.91	-6.45	-5.43	-5.61
Zr	-5.74	-5.33	-4.75	-3.72	-1.88	-1.48
Nb	-8.09	-7.48	-6.04	-5.77	-4.52	-6.10
Mo	-5.37	-4.89	-3.85	-3.11	-1.43	-2.18
Tc	-4.61	-4.21	-3.41	-2.19	-0.03	-0.09
Ru	-3.41	-3.22	-2.88	-1.62	0.32	0.62
Rh	-5.39	-5.11	-4.63	-3.72	-2.31	-2.42
Pd	-6.38	-6.06	-5.46	-5.18	-4.72	-5.29
Ag	-7.46	-6.98	-6.16	-6.00	-5.62	-6.10
Cd	-7.86	-7.34	-6.46	-6.35	-6.12	-6.50

Hf	-6.78	-6.13	-5.56	-4.56	-2.69	-2.33
Ta	-8.39	-7.68	-6.25	-6.08	-4.85	-6.59
W	-4.75	-4.20	-3.20	-2.50	-0.78	-1.58
Re	-2.95	-2.59	-2.05	-0.85	1.23	1.22
Os	-3.21	-2.93	-2.52	-1.25	0.83	0.98
Ir	-4.43	-4.12	-3.73	-2.78	-1.34	-1.52
Pt	-7.74	-7.23	-6.42	-6.06	-5.38	-6.21
Au	-7.60	-7.07	-6.32	-6.13	-5.76	-6.28
Hg	-3.31	-2.91	-2.57	-2.02	-1.33	-0.78

*Formation energy (E_f), $E_f = E_{\text{catalyst}} - E_v - E_m$ where E_{catalyst} , E_v , and E_m represent the DFT energy of SAA catalyst, the DFT energy of SAA catalyst with a TM vacancy, and the DFT energy of a TM atom in their corresponding metal bulk, respectively.

Table S3. Gibbs free energy changes of NORR on TM/Cu(111).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-1.21	-0.65	-0.62	0.30	-1.82	-1.22	1.19
Ti	-2.15	0.19	0.09	-2.00	-0.89	-0.59	1.31
V	-3.04	0.31	-0.64	-1.26	-0.31	-0.40	1.29
Cr	-3.46	0.59	-0.98	-0.70	-0.12	-1.59	2.22
Mn	-1.89	0.93	-1.09	-0.56	-0.26	-0.61	-0.54
Fe	-2.41	1.16	-0.96	-0.37	-0.75	-0.74	0.02
Co	-2.96	0.96	-1.06	0.19	-1.15	-0.98	0.96
Ni	-2.07	0.64	-0.82	-1.17	-0.72	-0.69	0.78
Cu	-0.76	-0.01	-0.50	-1.51	-0.22	-1.41	0.37
Zn	-0.47	-0.12	-0.65	-1.46	-0.93	-0.71	0.31
Y	-0.91	0.66	-2.18	1.05	-2.21	-1.49	1.05
Zr	-1.73	0.40	-1.64	-0.21	-1.35	-0.84	1.33
Nb	-2.74	0.41	-0.38	-1.42	-0.62	-0.67	1.38
Mo	-3.19	0.58	-0.92	-0.71	-0.38	-0.72	1.31
Tc	-3.35	0.98	-1.18	-0.38	-0.54	-0.97	1.40
Ru	-2.92	1.13	-0.96	-0.18	-0.98	-1.14	1.01
Rh	-2.00	0.82	-0.03	-0.47	-1.65	-1.47	0.77
Pd	-1.01	0.32	-0.71	-1.30	0.04	-1.69	0.31
Ag	-0.42	-0.34	-0.80	-1.24	0.51	-1.88	0.13
Cd	-0.27	1.19	-2.46	-1.24	-0.69	-0.78	0.22

Hf	-1.83	0.37	-1.36	-0.47	-1.35	-0.80	1.41
Ta	-2.66	0.13	-1.17	-0.73	-0.57	-0.49	1.46
W	-3.33	0.34	-0.70	-1.08	-0.27	-0.42	1.43
Re	-3.55	0.82	-1.25	-0.57	-0.18	-0.60	1.30
Os	-3.18	1.04	-1.22	-0.11	-0.76	-0.97	1.16
Ir	-2.39	1.04	-0.76	-0.32	-1.24	-1.19	0.84
Pt	-1.12	0.39	-0.79	-1.21	-0.24	-1.52	0.45
Au	-0.56	1.33	-2.21	-1.26	0.43	-1.86	0.10
Hg	-0.21	1.26	-2.49	-1.28	0.62	-1.87	-0.07

Table S4. Gibbs free energy changes of NORR on TM/Cu(100).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-1.20	0.51	1.07	-2.66	-1.91	-0.95	1.01
Ti	-2.18	0.03	0.16	-2.00	-0.90	-0.45	1.30
V	-3.08	0.28	-0.60	-1.27	-0.32	-0.32	1.27
Cr	-2.15	0.61	-1.03	-0.73	-0.18	-0.44	-0.13
Mn	-1.97	0.91	-1.22	-0.45	-0.36	-0.54	-0.42
Fe	-3.42	1.27	-1.25	-0.35	-0.78	-0.58	1.08
Co	-2.92	1.07	-0.59	-0.57	-1.09	-0.87	0.93
Ni	-1.96	0.74	0.04	-0.98	-1.41	-1.14	0.67
Cu	-0.87	-0.61	-1.26	1.61	-2.66	-0.57	0.33
Zn	-0.41	-1.06	-1.23	-1.01	0.76	-1.43	0.35
Y	-0.93	0.81	1.23	-2.62	-2.33	-1.15	0.95
Zr	-1.80	0.17	0.51	-2.31	-1.18	-0.59	1.18
Nb	-2.80	0.30	-0.34	-1.55	-0.44	-0.53	1.33
Mo	-3.27	0.62	-0.96	-0.73	-0.40	-0.61	1.31
Tc	-3.34	1.03	-1.33	-0.52	-0.52	-0.79	1.43
Ru	-2.82	1.30	-1.39	-0.09	-1.10	-0.92	0.98
Rh	-1.89	1.01	-0.66	-2.23	0.38	-1.28	0.63
Pd	-0.89	-0.37	1.60	-3.79	0.86	-1.63	0.18
Ag	-0.41	-0.74	2.74	-4.97	1.06	-1.72	0.00
Cd	-0.26	-0.87	3.00	-5.29	0.94	-1.69	0.12

Hf	-1.89	0.30	0.49	-2.41	-1.34	-0.56	1.38
Ta	-2.79	0.17	-1.82	-0.18	-0.58	-0.27	1.44
W	-3.38	0.44	-0.88	-1.10	-0.21	-0.32	1.41
Re	-3.60	0.83	-1.32	-0.58	-0.24	-0.48	1.35
Os	-3.16	1.24	-1.62	-0.25	-0.66	-0.76	1.17
Ir	-2.36	1.20	-1.24	-0.19	-1.24	-0.97	0.76
Pt	-1.26	-0.07	0.79	-2.96	0.50	-1.38	0.34
Au	-0.53	-0.50	2.12	-4.34	0.84	-1.58	-0.04
Hg	-0.25	-0.74	2.84	-5.04	0.92	-1.61	-0.16

Table S5. Gibbs free energy changes of NORR on TM/Cu(110).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-1.34	0.54	-2.23	0.65	-1.95	-0.76	1.06
Ti	-2.22	0.15	-0.01	-1.97	-0.95	-0.24	1.21
V	-2.97	0.29	-0.73	-1.14	-0.58	-0.14	1.22
Cr	-3.33	0.55	-1.06	-0.66	-0.50	-0.14	1.11
Mn	-3.49	0.91	-1.19	-0.50	-0.54	-0.34	1.11
Fe	-2.36	1.18	-1.01	-0.45	-0.93	-0.45	-0.01
Co	-2.86	1.47	-0.76	-0.74	-1.22	-0.71	0.78
Ni	-1.96	1.31	-0.36	-1.22	-1.59	-0.87	0.66
Cu	-0.86	1.06	0.32	-1.64	-2.07	-1.18	0.33
Zn	-0.62	0.98	0.61	-3.33	-0.85	-1.11	0.28
Y	-1.04	0.70	-2.73	1.31	-2.22	-0.91	0.84
Zr	-1.91	0.30	0.23	-2.19	-1.19	-0.44	1.16
Nb	-2.76	0.41	-0.58	-1.40	-0.72	-0.18	1.2
Mo	-3.19	0.57	-1.05	-0.76	-0.43	-0.42	1.24
Tc	-3.23	0.96	-1.35	-0.42	-0.63	-0.58	1.21
Ru	-2.76	1.36	-1.35	-0.22	-1.07	-0.76	0.76
Rh	-1.81	1.22	-0.74	-0.52	-1.52	-1.16	0.49
Pd	-0.77	-0.11	1.31	-1.20	-1.90	-1.48	0.11
Ag	-0.42	1.20	0.78	-1.84	-2.20	-1.59	0.03
Cd	-0.41	1.19	0.94	-2.04	-2.44	-1.41	0.13

Hf	-1.86	0.24	-1.75	-0.16	-1.43	-0.41	1.33
Ta	-2.71	0.03	-0.33	-1.67	-0.74	-0.04	1.42
W	-3.29	0.25	-0.97	-0.99	-0.43	0.05	1.33
Re	-3.52	0.74	-1.37	-0.56	-0.41	-0.12	1.2
Os	-3.13	1.10	-1.48	-0.26	-0.71	-0.49	0.93
Ir	-2.27	1.21	-1.21	-0.30	-1.31	-0.70	0.55
Pt	-1.04	0.92	-0.40	-0.94	-1.68	-1.13	0.24
Au	-0.51	1.74	-0.21	-1.62	-2.00	-1.46	0.02
Hg	-0.34	1.14	0.78	-1.98	-2.15	-1.35	-0.14

Table S6. Gibbs free energy changes of NORR on TM/Cu(211).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-1.18	0.51	-2.09	0.48	-1.99	-0.80	1.04
Ti	-2.82	0.63	-1.70	-0.09	-0.90	-0.27	1.11
V	-2.88	0.22	-0.76	-1.03	-0.48	-0.19	1.09
Cr	-3.26	0.48	-1.05	-0.59	-0.33	-0.35	1.06
Mn	-1.64	0.77	-1.10	-0.40	-0.47	-2.04	0.84
Fe	-3.28	1.13	-0.99	-0.46	-0.84	-0.55	0.95
Co	-2.88	0.76	-0.07	-0.74	-1.25	-0.73	0.87
Ni	-2.13	1.51	-1.71	-1.11	-0.35	-1.07	0.81
Cu	-0.92	1.16	0.24	-3.51	-0.26	-1.22	0.47
Zn	-0.71	1.10	-1.81	-1.69	-0.20	-1.13	0.41
Y	-1.06	0.87	-2.29	-1.57	0.09	-0.96	0.88
Zr	-1.72	0.14	-1.83	0.01	-1.35	-0.35	1.05
Nb	-2.54	0.27	-0.62	-1.30	-0.62	-0.38	1.16
Mo	-3.00	0.41	-1.04	-0.70	-0.29	-0.56	1.14
Tc	-3.16	0.88	-1.28	-0.34	-0.52	-0.81	1.20
Ru	-2.77	1.35	-1.39	-0.18	-0.91	-0.94	0.81
Rh	-2.00	0.71	-0.09	-1.66	-0.35	-1.34	0.69
Pd	-0.92	1.25	0.13	-3.06	-0.15	-1.50	0.21
Ag	-0.46	1.27	0.88	-4.69	0.48	-1.61	0.09
Cd	-0.43	1.13	1.05	-4.57	0.04	-1.52	0.25

Hf	-1.83	0.21	-1.52	-0.35	-1.39	-0.38	1.22
Ta	-2.66	0.04	-0.90	-1.10	-0.64	-0.08	1.30
W	-3.35	0.27	-0.79	-1.07	-0.14	-0.21	1.26
Re	-3.45	0.61	-1.28	-0.58	-0.06	-0.40	1.12
Os	-3.27	1.26	-1.56	-0.30	-0.87	-0.31	1.01
Ir	-2.43	0.94	-1.17	-0.55	-0.62	-0.91	0.70
Pt	-1.30	0.49	-1.09	-0.80	-0.39	-1.33	0.38
Au	-0.71	1.28	-2.13	-1.35	0.34	-1.54	0.08
Hg	-0.34	1.19	-2.49	-1.30	0.25	-1.23	-0.11

Table S7. Gibbs free energy changes of NORR on TM/Cu(320).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-1.37	-0.41	-1.48	-0.63	-0.57	-0.61	1.04
Ti	-2.83	0.64	-1.80	-0.14	-0.90	-0.20	1.20
V	-2.94	0.21	-0.86	-1.16	-0.39	-0.11	1.20
Cr	-3.15	0.52	-1.26	-0.64	-0.41	-0.28	1.17
Mn	-1.40	0.88	-1.23	-0.44	-0.46	-2.22	0.83
Fe	-3.44	1.20	-1.10	-0.39	-0.89	-0.50	1.10
Co	-3.05	1.47	-0.76	-0.69	-1.45	-0.48	0.92
Ni	-2.39	1.50	-0.26	-1.05	-1.60	-1.14	0.91
Cu	-1.07	1.19	-2.49	-0.81	0.08	-1.57	0.64
Zn	-0.64	1.16	-2.77	1.32	-2.20	-1.48	0.57
Y	-1.07	0.80	-2.74	1.21	-2.35	-0.78	0.89
Zr	-2.70	0.93	-2.01	0.02	-1.43	-0.15	1.32
Nb	-2.79	0.21	-1.36	-0.61	-0.61	-0.20	1.33
Mo	-3.28	0.46	-1.18	-0.71	-0.36	-0.27	1.30
Tc	-3.33	0.75	-1.37	-0.28	-0.53	-0.49	1.22
Ru	-3.13	1.37	-1.46	-0.10	-0.89	-0.76	0.93
Rh	-2.27	1.32	-0.79	-0.55	-1.32	-1.06	0.64
Pd	-1.11	1.34	0.03	-1.22	-1.68	-1.60	0.21
Ag	-0.55	1.39	0.82	-1.96	-2.11	-1.68	0.06
Cd	-0.42	1.26	-2.98	1.81	-2.45	-1.41	0.15

Hf	-2.48	0.87	-1.94	-0.14	-1.47	-0.23	1.35
Ta	-2.97	0.04	-0.43	-1.69	-0.60	0.18	1.43
W	-3.54	0.22	-0.98	-1.21	-0.02	0.10	1.40
Re	-3.73	0.45	-1.25	-0.56	-0.20	-0.01	1.26
Os	-3.59	1.17	-1.63	-0.32	-0.54	-0.37	1.24
Ir	-2.80	0.95	-0.99	-0.26	-0.95	-0.81	0.82
Pt	-1.55	1.15	-0.50	-0.79	-1.45	-1.27	0.38
Au	-0.67	1.29	0.35	-1.61	-2.00	-1.44	0.05
Hg	-0.26	1.19	0.75	-1.90	-2.26	-1.42	-0.14

Table S8. Gibbs free energy changes of NORR on TM/Cu(553).

	ΔG^*_{NO}	ΔG^*_{NOH}	ΔG^*_{N}	ΔG^*_{NH}	$\Delta G^*_{\text{NH}_2}$	$\Delta G^*_{\text{NH}_3}$	NH ₃ desorption
Sc	-2.09	1.56	-2.27	-1.48	0.14	-1.01	1.12
Ti	-2.72	0.71	-1.67	-0.21	-0.84	-0.58	1.28
V	-2.78	0.04	-0.60	-1.11	-0.42	-0.45	1.29
Cr	-3.38	0.54	-0.95	-0.73	-0.48	-0.38	1.35
Mn	-3.52	0.85	-1.19	-0.47	-0.63	-0.27	1.20
Fe	-3.34	1.11	-0.94	-0.53	-0.69	-0.76	1.13
Co	-2.93	1.23	-0.57	-1.59	-0.25	-0.93	1.00
Ni	-2.20	1.02	0.10	-2.39	-0.23	-1.08	0.75
Cu	-1.02	0.14	-0.83	-1.32	0.07	-1.53	0.46
Zn	-0.70	-0.09	-0.85	-1.41	0.05	-1.39	0.35
Y	-0.92	0.83	-2.43	-1.52	0.27	-1.19	0.91
Zr	-2.42	0.87	-1.82	-0.08	-1.25	-0.49	1.16
Nb	-2.54	0.24	-1.54	-0.55	-0.48	-0.44	1.28
Mo	-3.10	0.51	-0.96	-0.97	-0.31	-0.48	1.27
Tc	-3.24	0.79	-1.26	-0.45	-0.43	-0.86	1.42
Ru	-2.86	1.09	-1.24	-0.22	-0.76	-1.13	1.10
Rh	-2.12	1.16	-0.58	-1.45	-0.46	-1.35	0.77
Pd	-1.17	0.75	-1.56	-0.77	0.01	-1.53	0.23
Ag	-0.59	0.42	1.82	-4.32	-1.02	-0.49	0.16
Cd	-0.43	0.23	-1.24	-1.37	0.20	-1.58	0.15

Hf	-1.78	0.39	-1.78	-0.22	-1.48	-0.45	1.27
Ta	-2.62	-0.01	-0.23	-1.80	-0.76	-0.04	1.42
W	-3.38	0.23	-0.78	-1.22	-0.34	-0.02	1.47
Re	-3.61	0.58	-1.20	-0.67	-0.27	-0.15	1.28
Os	-3.27	0.88	-1.37	-0.39	-0.47	-0.62	1.20
Ir	-2.40	1.03	-1.10	-0.51	-0.95	-0.92	0.82
Pt	-1.38	1.10	-0.45	-1.89	-0.60	-1.29	0.47
Au	-0.65	0.54	1.15	-3.57	-0.05	-1.51	0.06
Hg	-0.31	0.29	1.82	-4.18	-0.06	-1.50	-0.10

Table S9. The distance between the N atom of NH₃ from the nearest surface atom in the IS, TS and FS structures (Å).

Systems	IS	TS	FS
Cd/Cu(553)	2.424	4.409	6.294
Zn/Cu(111)	2.269	4.281	6.147
Cu/Cu(111)	2.172	4.770	7.336
V/Cu(553)	2.185	4.124	6.723
Cu/Cu(553)	2.182	4.235	6.938
Zn/Cu(553)	2.266	4.480	6.989
Nb/Cu(553)	2.341	4.459	6.869
Ta/Cu(553)	2.308	4.456	6.857
W/Cu(553)	2.275	4.438	6.894
Sc/Cu(111)	2.351	6.240	8.010
Ta/Cu(111)	2.297	5.331	8.199
Ti/Cu(111)	2.225	6.124	8.092
Nb/Cu(100)	2.329	4.798	7.395
Ti/Cu(100)	2.227	4.736	7.314
Ta/Cu(100)	2.294	4.898	7.434
V/Cu(100)	2.149	4.769	7.374
V/Cu(110)	2.164	6.154	9.011
Zr/Cu(110)	2.416	6.844	8.911
Hf/Cu(110)	2.349	6.626	9.009

Ta/Cu(110)	2.300	6.633	9.058
W/Cu(110)	2.264	6.627	9.095
Zr/Cu(211)	2.429	5.390	6.897
Ti/Cu(110)	2.252	6.566	7.351
V/Cu(211)	2.197	4.581	7.005
W/Cu(211)	2.282	4.699	7.102
Nb/Cu(211)	2.351	4.666	7.012
Hf/Cu(211)	2.362	4.678	6.999
Ta/Cu(211)	2.314	4.662	7.059
Sc/Cu(320)	2.367	5.442	6.674
V/Cu(320)	2.168	5.253	6.784
Nb/Cu(320)	2.330	5.386	6.790
Ta/Cu(320)	2.289	5.573	6.824
W/Cu(320)	2.253	5.423	6.857

Table S10. Frequencies of IS, TS and FS for NH₄⁺ formation on the 33 screened catalysts (cm⁻¹).

	IS	TS	FS		IS	TS	FS
Sc/Cu(111)	51.20	-1100.99	46.00	Ti/Cu(111)	49.35	-1089.42	44.02
	53.50	51.09	51.24		58.41	47.50	49.27
	65.69	53.37	52.17		60.51	49.27	57.84
	67.30	66.14	56.41		61.12	58.93	60.11
	67.61	66.98	66.79		66.90	60.16	60.34
	68.09	67.20	67.42		67.19	60.51	64.33
	68.95	67.92	67.97		68.72	66.94	67.20
	70.52	68.01	68.09		69.33	67.23	68.09
	71.90	69.82	70.07		73.26	68.31	68.69
	72.88	71.14	71.17		73.71	68.87	69.04
	74.73	72.27	71.50		74.50	73.51	74.16
	75.13	72.91	73.84		74.73	73.95	74.85
	76.46	74.91	74.55		75.55	74.60	75.16
	76.94	74.97	75.36		75.93	75.05	75.86
	88.59	76.63	75.80		83.12	75.59	76.38
	88.75	77.92	77.10		84.80	76.00	77.56
	89.12	88.19	78.29		85.70	84.57	84.45
	89.89	88.95	89.37		88.77	84.95	85.38
	90.92	89.61	90.02		89.42	88.21	88.02
	92.46	90.94	90.40		90.48	90.20	89.79
	93.94	92.11	91.05		92.10	92.38	92.40
	97.55	93.49	91.78		93.05	92.78	92.74
	97.60	94.86	93.42		93.30	93.24	93.29
	98.30	96.73	96.33		96.02	95.57	95.55
	99.34	97.04	96.78		97.52	96.78	96.50
	102.41	97.84	97.56		98.48	98.11	98.11
	103.08	98.90	98.86		99.08	100.23	100.46
	103.35	102.05	100.94		100.86	100.78	100.98
	104.38	102.84	102.16		101.12	101.25	101.93
	104.57	102.98	103.44		103.14	103.28	103.45
	105.09	104.36	104.10		103.71	103.66	104.04
	105.93	104.57	104.76		104.19	104.08	104.37
	106.42	105.75	105.14		104.67	104.95	105.30
	107.18	105.99	105.94		105.56	105.27	105.88
	107.83	106.67	106.38		105.72	105.44	106.00
	108.45	107.05	107.10		106.17	106.24	106.46
	109.27	108.01	107.19		106.30	106.40	106.71
	111.37	108.18	108.22		106.74	106.67	106.90
	112.56	109.71	108.38		106.85	107.07	107.23
	113.84	110.63	109.81		109.47	109.00	108.60
	116.09	111.94	111.06		110.04	109.97	110.47

116.41	114.49	112.95	110.98	110.88	111.57
117.51	115.88	114.89	112.44	112.14	112.91
119.14	115.92	115.99	116.26	115.71	115.29
120.89	117.04	116.24	117.00	116.88	116.06
121.56	119.61	116.63	117.04	117.05	116.63
122.43	120.67	120.43	118.59	117.99	117.28
123.32	121.96	121.85	120.32	119.48	119.13
123.88	122.47	121.98	120.56	120.59	119.48
124.37	123.37	122.19	120.81	121.43	121.10
124.80	123.48	123.16	121.86	122.12	122.23
124.96	124.13	123.35	123.00	122.83	122.90
125.23	124.55	123.67	123.17	123.26	123.44
125.62	124.65	124.27	123.88	123.94	123.86
125.94	125.00	124.59	124.02	124.18	123.93
126.17	125.31	125.14	124.44	124.76	124.64
126.24	125.93	125.41	125.56	125.50	124.97
128.38	126.06	125.64	126.84	125.91	125.94
128.53	126.09	125.92	127.17	126.72	126.15
129.36	128.22	126.00	127.71	127.61	127.14
129.53	128.36	127.76	128.14	127.82	127.49
129.84	129.04	128.14	128.39	128.26	128.16
130.65	129.46	128.70	128.79	128.51	128.37
131.10	129.78	129.02	129.47	128.98	128.86
131.60	130.15	129.75	129.66	129.20	129.02
133.49	130.67	129.80	129.91	129.47	129.19
133.99	131.08	130.16	130.35	130.20	129.26
134.41	133.15	130.87	131.06	130.67	130.17
134.62	133.50	132.65	131.77	131.47	130.42
134.83	134.08	133.04	132.79	132.52	131.36
135.53	134.28	133.73	134.88	134.55	132.69
136.05	134.43	133.96	135.17	135.06	134.61
136.96	135.84	134.18	135.83	136.20	134.98
138.06	136.62	135.84	137.61	137.39	136.63
138.73	136.85	136.86	137.73	137.60	137.66
139.15	138.72	138.57	138.34	137.98	137.91
139.87	139.34	138.65	138.88	138.47	138.37
141.39	139.78	139.35	139.74	139.16	138.61
142.10	141.34	139.82	140.39	139.96	139.36
142.50	141.90	141.33	140.58	140.24	140.05
142.91	142.40	141.76	141.15	141.05	140.24
145.62	142.51	142.20	141.47	141.32	141.09
145.68	145.23	142.40	142.63	142.33	141.45
146.61	145.46	144.68	143.83	143.28	142.35
146.84	146.39	145.02	144.02	143.73	143.04

148.77	146.56	146.14	144.40	144.11	143.39
149.65	148.63	146.43	145.52	144.77	144.03
149.74	149.03	148.29	146.18	145.72	144.59
150.02	149.25	148.62	147.05	146.63	145.50
150.12	149.45	148.84	147.58	147.05	146.50
150.41	149.50	149.24	147.82	147.28	146.82
150.64	150.23	149.35	149.56	149.11	147.24
151.18	150.60	149.65	150.62	149.67	148.96
152.32	151.06	150.51	151.19	149.97	149.48
152.67	151.89	150.61	151.56	150.26	149.84
153.61	152.07	151.49	152.38	151.53	150.35
153.78	153.01	151.60	152.75	152.13	151.62
154.67	153.36	152.44	155.03	154.42	152.05
155.11	154.08	152.80	155.23	154.83	154.24
156.12	154.74	153.53	156.38	155.88	154.76
156.59	154.90	154.07	156.61	156.47	155.53
158.03	154.96	154.27	157.24	156.80	156.29
160.65	158.43	155.53	157.43	157.19	156.72
160.82	159.81	158.47	158.26	157.30	157.01
162.54	159.95	159.74	158.74	157.76	157.08
162.66	160.43	159.85	158.90	158.34	157.73
162.84	161.61	161.04	161.33	160.33	158.22
163.99	163.67	161.55	162.18	161.15	160.54
164.67	163.80	163.13	163.52	162.77	161.42
166.16	166.03	163.33	164.29	163.70	162.51
166.73	166.49	165.70	164.71	164.15	163.52
167.82	167.69	166.02	167.36	166.60	163.97
169.77	169.91	167.37	167.86	166.87	166.44
170.66	170.35	169.28	170.15	169.78	166.74
171.15	170.63	169.93	171.18	170.35	169.90
171.78	171.12	170.72	172.45	171.89	170.39
172.23	171.42	170.97	173.21	172.39	171.75
173.37	172.45	171.21	173.47	173.05	172.59
173.85	173.60	172.62	173.56	173.26	172.96
174.72	174.18	173.30	174.05	173.87	173.21
175.65	175.05	173.88	174.79	174.21	173.81
176.18	175.20	174.44	175.71	175.34	174.00
176.43	176.00	175.17	176.09	175.41	175.12
177.06	176.67	175.39	177.00	176.52	175.50
177.42	177.33	176.54	177.27	176.99	176.30
179.12	178.20	177.80	177.65	177.76	176.91
181.13	178.95	178.27	178.36	177.91	177.72
181.24	181.07	180.44	181.68	180.50	178.10
182.92	181.98	180.68	182.41	180.98	180.45

183.20	182.32	181.72	182.96	181.89	181.38
184.00	183.55	182.16	184.28	184.02	181.73
184.73	184.06	183.24	184.77	184.42	183.86
185.41	184.96	183.47	186.32	185.81	184.23
187.51	186.30	184.56	186.93	186.55	185.72
187.99	187.19	185.89	188.36	186.96	186.53
190.98	189.70	186.82	189.55	188.65	187.80
191.08	190.27	189.29	189.74	188.95	188.30
191.85	190.76	190.37	189.96	189.56	188.59
192.43	191.48	190.70	190.38	189.67	189.36
192.71	191.70	191.22	192.75	192.43	189.43
192.96	192.00	191.42	192.95	192.60	192.13
194.47	193.00	192.40	193.76	193.35	192.45
195.23	194.48	193.76	194.04	193.48	193.15
196.90	194.76	194.09	196.54	194.62	193.27
204.95	195.39	194.57	202.55	195.53	193.86
205.89	203.18	202.42	203.49	200.86	198.99
206.75	204.64	203.34	203.60	202.17	200.88
207.86	205.25	203.55	204.35	203.16	201.37
210.77	207.62	205.36	210.12	208.80	203.01
212.86	210.29	209.51	210.81	210.41	209.12
215.13	212.52	212.14	212.97	210.80	210.09
215.63	215.09	214.34	215.09	212.98	212.08
216.57	215.40	214.81	216.33	214.73	214.54
216.84	216.00	215.08	216.67	216.16	215.74
217.52	216.44	215.68	216.94	216.30	215.84
217.66	217.32	216.39	217.27	216.71	216.16
218.18	217.43	216.59	218.22	216.93	216.36
218.59	217.93	217.26	218.91	217.79	217.29
219.23	218.22	217.38	219.16	218.49	218.06
220.68	219.30	218.56	220.60	218.83	218.44
221.56	220.77	219.75	221.31	220.45	220.22
221.86	221.65	220.57	221.34	221.11	220.59
222.37	221.73	220.76	221.99	221.32	220.84
222.98	222.81	221.45	222.13	221.68	221.34
229.34	223.22	222.17	225.85	221.86	221.46
230.50	227.29	226.90	226.64	223.94	222.71
232.92	228.92	228.21	233.65	225.02	223.23
233.17	232.96	232.36	234.38	233.58	233.27
236.01	233.19	232.68	234.73	233.98	233.33
236.23	235.76	235.09	235.61	234.15	233.79
238.14	236.27	235.56	235.99	234.71	234.18
238.50	237.02	236.40	236.46	235.13	234.35
240.10	238.17	237.29	239.67	235.56	234.95

	241.62	239.92	239.46		240.44	238.96	238.42
	242.05	241.61	240.83		242.48	239.32	238.75
	244.00	241.81	240.95		243.38	241.78	241.52
	244.44	242.51	241.53		243.62	242.77	242.39
	247.07	243.07	242.06		244.34	243.08	242.64
	248.36	246.47	245.63		244.94	243.59	243.18
	249.32	247.64	246.55		248.06	243.98	243.48
	250.29	249.03	247.04		248.99	247.61	247.38
	251.77	249.29	248.19		249.15	248.42	248.08
	253.08	249.97	248.82		250.27	248.90	248.30
	254.00	251.06	249.59		251.42	249.41	248.94
	254.80	252.22	251.25		253.04	250.97	250.81
	257.21	253.77	252.73		253.73	252.69	252.20
	259.83	256.90	255.56		254.11	253.42	252.89
	261.15	259.11	257.38		256.04	253.76	253.34
	261.70	259.64	258.07		257.33	255.94	255.44
	262.10	259.98	258.47		257.88	256.77	256.37
	270.45	262.02	260.20		266.72	257.35	257.01
	523.92	270.51	268.91		492.05	266.34	265.95
	528.00	311.30	333.25		515.10	316.52	376.62
	759.31	422.02	483.07		895.44	445.17	489.96
	3537.30	3550.21	3514.92		3548.08	3575.38	3528.72
Cu/Cu(111)	49.51	-1231.46	48.97	Zn/Cu(111)	49.58	-1169.50	48.59
	53.69	48.33	53.44		53.58	53.81	49.23
	67.80	49.23	64.60		68.22	69.73	54.50
	69.45	49.38	69.75		69.88	70.11	65.73
	70.07	53.76	70.12		70.50	70.44	70.07
	70.40	69.48	70.71		70.61	70.85	70.49
	71.86	70.03	71.35		71.59	71.10	70.95
	72.04	70.78	72.43		72.48	72.63	72.05
	76.14	71.03	74.15		75.60	75.25	73.05
	76.91	71.98	77.40		76.38	76.83	73.82
	76.95	72.55	77.66		76.87	77.62	76.97
	77.28	76.57	78.03		77.57	77.99	77.73
	78.38	77.38	78.57		78.58	78.25	78.08
	78.74	77.61	78.84		78.61	79.00	78.77
	90.68	77.72	83.83		90.29	91.71	78.83
	91.26	78.88	89.24		91.56	92.49	81.99
	93.60	79.11	91.91		94.23	93.43	91.31
	94.56	91.98	94.05		94.73	93.85	93.31
	95.92	93.59	95.11		95.61	95.75	94.41
	96.41	94.02	96.48		96.14	96.52	96.11
	96.72	96.15	96.75		96.62	97.00	96.36
	98.14	96.47	97.40		97.28	98.14	97.02

100.92	96.69	98.20	98.04	99.93	97.63
101.35	96.85	98.70	100.97	101.34	97.70
101.74	98.21	101.51	102.19	102.14	100.68
102.22	100.90	101.94	102.53	102.49	102.29
102.71	101.27	103.36	102.82	103.39	102.63
103.54	102.07	104.02	103.78	103.81	103.32
105.02	102.86	104.84	104.49	105.77	104.36
106.50	103.65	106.46	106.37	106.20	104.78
106.72	104.53	107.42	106.79	107.29	106.57
107.53	106.02	107.78	107.17	107.98	107.47
107.87	106.68	108.74	108.01	108.56	107.93
108.98	107.28	109.26	108.80	109.14	108.74
109.24	108.37	110.01	108.96	109.86	109.12
110.41	108.52	110.37	110.56	110.85	109.63
110.98	109.28	111.31	111.15	111.12	110.62
112.67	109.45	112.07	112.84	113.24	110.97
114.00	111.05	112.72	113.56	114.08	111.71
114.85	111.15	113.52	114.14	114.35	113.10
115.07	113.21	114.89	114.76	115.23	113.62
119.36	113.94	116.40	118.96	119.07	115.38
120.93	115.28	116.84	119.37	120.74	115.80
121.72	115.85	121.19	121.33	121.57	120.02
122.61	120.70	122.72	122.35	122.42	120.73
123.84	122.66	123.65	122.52	123.04	122.41
124.10	123.07	124.00	123.47	124.17	123.12
124.68	123.57	125.61	124.15	124.71	123.38
125.05	125.12	125.91	124.93	125.44	124.30
126.09	125.52	126.14	125.88	125.72	125.51
126.18	125.65	126.22	126.03	126.24	125.88
126.47	126.23	126.62	126.41	126.60	126.23
126.79	126.29	126.75	126.59	126.73	126.49
127.09	126.37	127.24	127.04	127.25	126.57
127.87	126.75	127.51	127.55	127.72	126.74
127.95	126.99	127.82	128.19	128.31	127.34
128.75	127.31	128.04	128.46	128.40	127.73
129.01	127.39	128.40	129.11	128.58	127.97
129.24	128.09	128.64	129.45	129.34	128.53
129.66	128.45	128.74	129.76	130.35	128.82
129.97	128.96	129.31	129.85	130.42	129.12
132.04	129.19	129.70	131.74	131.54	129.44
132.50	129.46	130.20	132.38	131.94	130.13
132.84	129.72	131.84	133.10	132.47	131.21
132.99	131.87	132.30	133.31	132.98	131.75
133.44	132.07	132.44	133.59	133.55	132.17

135.39	132.29	132.87	134.83	133.95	133.21
135.52	132.87	133.15	135.32	135.47	133.37
135.79	132.94	135.92	136.15	136.63	134.98
136.43	134.56	136.06	136.53	136.78	135.75
136.80	135.68	136.47	137.30	137.08	136.05
137.44	135.94	136.59	137.55	137.41	136.93
140.02	136.26	138.39	139.55	139.21	137.08
142.28	136.83	138.84	142.16	141.06	138.28
143.01	137.70	141.97	142.84	143.52	140.86
144.37	140.19	143.74	143.40	144.05	142.56
144.55	143.72	143.99	144.56	144.24	143.55
144.81	144.19	144.45	144.83	144.62	144.07
145.29	144.35	144.96	145.44	145.25	144.53
145.66	144.76	145.28	145.81	145.71	145.15
146.21	144.96	145.45	146.92	146.27	145.42
146.70	145.29	145.63	147.03	147.10	145.93
147.19	145.47	146.34	147.80	147.44	146.01
148.20	145.82	146.52	148.48	148.13	146.52
148.96	146.36	147.35	148.89	148.98	147.59
149.81	146.62	147.74	149.83	149.52	147.85
150.08	147.48	148.57	150.39	150.44	148.24
150.86	147.90	150.26	151.15	150.69	149.20
152.03	150.40	150.50	151.97	151.57	149.46
152.43	150.60	150.71	152.71	152.31	150.04
152.94	151.14	151.29	153.03	152.65	151.08
153.13	151.22	151.61	153.23	152.98	151.80
153.51	151.44	151.69	153.67	153.37	152.03
153.78	152.07	152.18	154.45	153.82	152.11
154.62	152.63	152.76	154.49	154.18	152.55
156.06	153.09	152.89	156.28	154.87	153.05
156.24	153.35	154.94	156.65	155.78	153.67
156.52	154.85	155.33	157.14	156.38	154.45
156.76	155.08	155.87	157.19	157.16	154.99
157.01	155.73	156.21	157.29	157.17	156.07
157.33	156.01	156.39	157.57	157.21	156.60
157.49	156.38	156.49	158.32	157.77	156.76
160.72	156.56	156.82	160.77	159.19	156.90
161.09	156.86	157.06	161.11	161.59	157.26
163.49	157.15	161.34	164.04	161.89	157.84
163.56	161.17	161.70	164.44	164.25	160.91
164.55	161.58	163.16	164.92	164.69	161.30
165.56	163.03	163.49	165.85	165.34	163.60
170.37	163.34	164.04	169.77	165.97	163.92
170.90	164.30	165.18	170.65	170.03	164.70

172.43	165.11	169.87	171.43	170.27	165.49
173.33	170.08	170.63	172.28	171.59	169.38
173.50	170.42	171.63	172.96	171.85	169.70
173.83	171.36	172.07	173.55	172.98	171.23
173.98	172.94	172.88	174.11	173.56	171.32
174.71	173.26	173.43	174.15	173.95	172.47
174.87	173.94	174.03	174.83	174.12	173.00
175.32	174.03	174.57	175.04	175.04	173.09
175.67	174.52	174.63	175.33	175.11	173.70
175.76	174.76	174.95	175.61	175.66	174.52
175.95	174.90	175.09	175.97	175.98	175.00
176.08	175.26	175.19	176.46	176.34	175.31
176.51	175.29	175.45	176.67	176.63	175.39
176.70	175.51	175.70	177.14	177.13	175.67
176.95	175.64	175.94	178.23	177.25	175.89
177.94	176.14	176.52	178.66	178.12	175.98
178.17	176.31	176.63	179.01	178.38	176.18
182.57	176.91	177.35	182.63	178.85	177.12
183.40	177.50	177.52	183.28	182.41	177.92
183.92	177.68	181.99	183.93	183.15	178.39
184.95	182.77	182.75	184.21	183.52	180.58
185.20	182.99	183.56	184.97	184.95	182.70
186.37	184.31	184.37	186.04	185.67	183.01
191.69	184.48	185.06	191.65	186.28	184.24
191.80	185.47	185.93	192.26	191.93	184.63
193.25	186.24	191.63	193.42	192.82	185.79
193.74	191.86	192.07	193.67	193.41	191.75
194.66	191.99	193.43	194.98	193.94	192.58
195.11	193.65	193.71	195.66	194.75	193.21
195.61	193.79	194.02	195.88	195.58	193.52
196.11	194.17	194.19	196.59	195.61	194.16
196.41	194.32	194.85	196.66	196.33	194.68
197.16	195.13	195.57	197.05	196.79	195.32
197.54	195.61	196.40	197.76	197.21	195.59
198.59	196.37	196.63	199.08	197.64	196.29
204.89	196.70	196.76	203.87	199.06	196.85
209.28	196.85	196.85	209.63	203.59	196.97
214.13	197.09	202.83	212.73	209.67	197.99
215.24	204.39	208.94	214.56	213.17	201.34
216.92	209.15	214.21	215.87	215.14	209.20
217.34	214.65	215.75	216.85	216.12	212.17
217.65	216.17	216.99	217.47	216.99	214.89
217.93	217.21	217.13	217.71	217.70	215.59
218.27	217.34	217.64	218.33	218.05	217.19

218.52	218.02	217.92		218.59	218.44	217.24	
219.05	218.19	218.08		218.98	218.61	218.07	
219.20	218.34	218.30		219.13	219.04	218.18	
219.60	218.77	218.90		219.49	219.12	218.51	
220.27	218.81	219.02		219.86	219.48	218.55	
220.61	219.21	219.06		220.73	219.75	218.68	
220.78	219.66	219.24		220.84	220.19	219.16	
220.92	219.80	219.60		221.41	220.75	219.29	
221.59	219.97	219.89		222.52	221.46	219.70	
222.22	220.22	220.15		223.31	222.43	220.14	
234.38	220.65	220.77		233.10	223.77	220.42	
234.85	220.80	221.13		233.83	233.55	221.59	
235.07	221.74	223.33		235.08	234.13	222.27	
235.41	234.48	234.36		235.48	235.16	233.54	
236.90	234.83	234.50		236.92	235.58	233.96	
237.07	235.08	234.74		238.01	236.65	234.81	
242.29	235.30	234.88		240.66	238.53	235.03	
243.15	236.81	236.44		241.69	241.11	236.36	
243.73	236.85	236.77		243.03	241.93	237.67	
243.97	242.51	241.98		244.17	243.30	241.30	
245.07	242.76	242.29		244.59	244.18	241.97	
245.27	243.57	243.09		245.98	244.52	242.70	
246.29	243.77	243.27		246.71	245.81	243.47	
246.73	244.56	244.02		247.00	246.77	243.96	
247.35	244.71	244.23		247.70	246.89	245.30	
247.64	245.99	245.94		248.15	247.81	245.58	
254.78	246.44	246.14		253.00	248.50	246.53	
255.66	247.00	246.82		254.67	252.99	247.06	
256.25	247.45	247.18		256.35	254.99	247.48	
256.84	254.81	254.06		256.83	255.41	249.05	
257.63	255.62	254.86		258.31	257.36	253.90	
257.75	255.74	255.29		258.65	257.85	255.66	
258.52	256.74	255.97		259.56	258.54	256.52	
258.83	256.82	256.35		259.81	259.48	256.99	
270.69	257.12	256.82		271.01	260.30	257.44	
377.30	257.87	257.22		377.48	270.90	257.92	
388.41	258.51	257.63		380.02	306.84	258.28	
485.93	270.16	268.94		502.72	443.29	259.37	
504.41	308.10	286.26		508.61	541.99	270.50	
516.00	547.81	481.94		579.74	579.34	425.49	
3532.78	3601.96	3529.72		3536.53	3519.95	3533.35	
Ta/Cu(111)	51.38	-1211.38	46.50	Ti/Cu(100)	52.86	-1781.35	54.87
	52.20	61.44	52.66		56.25	53.64	55.48
	62.23	66.82	61.43		56.26	56.42	57.33

67.23	67.16	67.57	57.67	56.51	57.91
67.48	68.83	68.86	60.97	60.23	61.03
68.89	72.14	70.18	61.12	60.53	61.26
74.99	74.52	74.60	61.71	61.02	61.39
75.56	74.88	75.73	61.72	61.40	62.01
76.42	76.50	76.67	63.81	62.17	63.51
76.88	78.45	77.13	63.83	63.78	63.99
79.55	78.90	79.82	64.46	64.11	64.38
79.90	79.47	79.96	65.68	65.64	65.39
80.88	80.92	80.34	77.36	68.15	80.15
81.24	81.24	81.40	79.05	78.08	80.36
82.32	84.30	82.20	79.05	78.61	80.40
90.71	89.69	90.05	79.93	79.24	80.99
92.84	92.91	91.47	80.22	79.82	82.41
93.97	94.09	94.10	81.07	80.97	82.54
95.21	94.21	94.56	83.33	81.79	82.61
97.61	97.00	97.15	83.34	82.20	83.04
98.22	98.17	97.84	83.62	82.57	83.59
102.48	102.58	99.91	83.64	83.65	83.88
105.35	104.95	103.16	87.33	84.87	87.16
106.32	106.36	105.03	87.36	87.42	87.45
107.49	107.05	105.70	88.22	87.99	87.63
108.12	107.85	106.76	88.24	88.35	88.06
108.86	108.65	108.31	93.00	88.86	91.70
109.53	109.37	109.11	93.02	92.23	91.88
110.05	109.44	109.42	95.04	92.79	94.39
110.10	110.03	109.93	96.61	94.14	96.38
110.80	110.57	111.42	97.09	96.34	96.50
111.92	111.91	111.87	97.10	96.73	96.54
112.82	112.41	112.63	98.47	97.05	98.06
113.32	112.84	113.29	98.76	98.18	98.61
113.67	113.17	113.73	104.86	98.71	104.96
114.29	113.75	113.91	106.89	104.60	106.75
114.86	114.51	114.42	107.10	106.24	107.85
115.21	115.22	114.92	107.10	106.86	107.92
116.36	115.91	115.13	107.34	107.21	108.75
118.81	118.77	115.97	108.26	108.14	109.47
120.09	119.99	118.56	108.26	108.50	109.61
121.22	120.33	119.73	108.57	108.58	110.70
121.37	121.54	120.93	108.70	108.62	113.35
124.53	124.06	121.27	114.06	113.07	114.20
126.17	125.24	124.11	114.75	113.49	114.26
127.54	126.88	124.58	114.76	114.28	114.89
128.15	127.56	127.32	114.84	114.77	115.18

128.97	128.21	128.05	115.42	114.93	116.97
129.06	128.62	128.51	116.86	116.24	117.15
129.98	129.00	128.85	117.14	116.45	117.19
130.73	130.13	129.32	117.15	116.60	117.71
130.83	130.33	130.02	117.73	117.14	117.80
130.96	130.74	130.49	118.07	117.23	118.20
131.23	131.17	130.97	118.84	117.71	119.33
131.37	131.33	131.14	118.84	119.18	119.46
131.69	131.52	131.47	134.06	119.23	133.94
131.91	131.75	131.72	134.85	134.05	134.35
134.57	134.74	132.02	134.86	134.43	134.40
135.29	135.36	133.56	134.90	134.60	134.53
135.72	135.86	134.47	136.53	134.69	135.43
136.32	136.39	135.24	136.97	135.84	135.48
136.74	136.86	135.63	137.29	136.52	136.67
137.83	137.93	136.64	137.30	136.65	136.90
138.38	138.52	136.80	137.53	136.89	137.19
139.41	138.94	137.72	138.36	137.19	137.59
141.45	140.53	138.15	138.40	137.54	137.86
141.70	141.34	138.56	138.40	138.20	138.42
142.25	142.15	141.28	138.59	138.33	138.48
142.57	142.30	141.82	139.34	138.57	139.02
142.66	142.62	141.97	140.69	138.76	140.21
143.20	142.75	142.36	140.70	140.52	140.26
143.79	143.65	142.47	141.16	140.85	140.36
143.93	143.96	143.38	141.73	140.88	141.33
144.96	144.44	143.93	141.87	141.54	141.63
145.14	145.52	144.35	141.98	141.60	141.64
145.91	146.05	145.02	141.98	141.77	141.92
146.25	146.58	145.28	142.13	141.87	142.00
146.92	147.06	145.89	142.60	142.28	142.11
147.83	148.81	146.49	142.94	142.53	142.30
150.00	150.21	147.11	143.15	142.67	142.83
151.09	151.12	148.44	143.15	142.73	142.87
151.79	151.75	150.32	143.43	142.97	142.95
152.33	152.60	151.13	144.01	143.02	143.45
153.22	153.47	151.70	144.71	143.47	144.77
154.05	154.41	152.25	144.71	144.62	144.77
155.26	155.31	153.21	145.38	144.83	145.03
155.71	155.55	153.59	145.39	145.00	145.03
156.71	156.63	155.05	145.58	145.04	145.28
156.81	157.14	155.98	145.78	145.44	145.85
157.81	157.79	156.55	146.81	145.81	146.61
158.44	158.70	157.01	147.81	146.65	146.85

158.55	159.04	157.66	147.82	146.88	146.86
160.39	160.20	158.25	148.52	147.06	148.83
161.07	161.04	158.76	150.60	148.65	149.40
161.45	162.14	160.02	151.24	149.91	149.63
162.30	162.40	160.79	151.25	150.27	151.69
163.21	163.41	161.16	152.08	150.71	152.32
164.12	164.29	161.71	153.62	152.62	152.50
164.37	165.00	163.45	153.63	153.12	153.06
165.32	165.49	164.11	156.14	153.38	153.24
166.15	166.80	164.24	156.22	153.61	153.75
167.10	166.85	164.89	161.25	154.64	160.73
167.46	167.90	166.24	164.13	157.42	161.98
167.63	168.24	166.57	165.53	162.91	164.20
168.79	169.26	167.30	165.55	164.50	164.48
169.33	169.87	167.48	170.45	164.99	170.10
170.56	170.39	168.63	170.90	166.56	170.38
172.07	172.04	169.07	171.53	170.65	170.68
173.44	173.47	170.15	171.53	171.12	170.89
173.66	174.82	171.78	171.92	172.15	172.12
175.69	176.56	173.14	171.93	172.50	172.34
178.36	178.25	173.39	173.33	172.70	172.36
178.58	178.88	175.23	174.28	172.93	172.48
180.00	180.65	178.04	175.52	173.42	173.50
181.45	181.53	178.75	175.57	176.05	176.65
181.86	181.96	179.87	179.41	176.54	177.68
183.10	184.02	181.13	179.50	179.04	178.64
183.86	184.59	181.94	179.51	179.50	179.18
184.65	184.77	182.34	179.59	179.63	179.24
184.75	185.14	183.39	186.19	179.73	180.39
185.67	186.35	184.35	187.52	185.50	184.97
185.88	186.66	184.56	188.25	188.13	187.62
187.39	187.58	185.09	189.91	188.39	187.94
187.95	187.95	185.98	190.07	188.95	188.00
188.23	188.46	187.09	190.08	189.69	188.57
188.76	188.82	187.62	192.09	189.75	188.93
189.37	189.28	187.98	194.15	191.12	190.26
189.68	189.85	188.64	194.53	192.54	192.19
190.40	190.37	188.87	195.76	194.07	193.19
191.04	190.88	189.51	195.82	194.86	193.69
192.59	192.55	189.94	196.20	195.08	193.94
194.07	194.28	190.63	196.77	195.51	195.03
196.63	196.20	192.31	197.61	196.78	196.21
196.99	196.76	193.63	197.62	196.82	196.27
197.73	197.66	196.41	198.02	197.40	196.44

197.99	198.67	196.59	198.11	197.50	197.00
198.82	199.14	197.60	208.49	197.60	197.06
199.80	199.60	198.08	208.83	208.78	208.36
199.97	200.02	198.62	209.40	208.89	208.77
200.32	200.98	199.66	209.41	209.24	208.90
202.72	202.88	199.81	213.73	209.42	208.97
202.91	204.62	199.87	215.49	213.33	212.72
205.34	205.89	202.71	215.93	215.39	214.72
206.38	206.62	202.77	215.93	215.52	215.09
207.08	207.20	205.71	218.07	216.06	215.11
208.00	209.03	206.19	218.08	217.12	216.43
214.25	215.09	206.62	221.45	217.19	216.45
214.88	215.76	207.68	222.08	221.44	221.34
215.79	216.90	213.97	222.08	221.98	221.92
217.54	221.79	214.65	222.63	222.04	221.92
221.87	222.17	216.04	222.99	222.62	222.03
222.43	222.27	221.51	223.21	222.97	222.13
222.55	223.35	221.98	224.55	223.30	222.52
223.95	225.75	222.14	224.56	223.40	223.44
226.17	226.50	223.42	225.49	224.28	223.57
226.44	226.70	224.28	225.50	225.69	225.54
226.87	226.99	225.81	233.14	226.28	226.41
227.16	227.21	226.37	233.31	227.46	226.70
227.80	228.68	226.73	235.31	229.95	226.85
228.31	229.73	226.96	239.43	234.57	234.80
229.53	230.11	227.76	239.59	239.24	238.95
229.73	230.99	229.16	239.59	239.38	239.01
230.73	231.37	229.31	240.17	239.55	239.04
231.35	232.72	230.09	240.69	240.14	239.73
232.54	233.21	230.45	240.71	240.20	240.35
232.85	242.30	231.98	240.72	240.42	240.38
242.39	243.09	232.08	242.03	240.74	240.84
243.27	244.42	242.22	242.03	241.89	241.56
244.39	245.89	242.77	242.06	242.10	241.57
245.51	245.94	244.11	242.56	242.37	242.35
245.66	246.30	244.82	248.74	242.80	242.51
245.96	250.82	244.93	248.99	248.52	248.30
250.95	251.47	245.30	249.00	248.94	249.00
251.03	251.89	250.44	250.35	249.05	249.01
252.06	252.76	250.59	250.55	250.12	249.82
252.87	253.50	251.75	250.56	250.23	250.01
253.45	255.34	252.49	250.57	250.40	250.03
255.35	255.60	252.76	251.61	250.54	250.04
255.40	256.30	254.81	252.71	251.59	251.31

	256.53	256.70	254.96		253.70	252.85	252.18
	257.08	259.46	255.77		253.70	253.13	252.94
	259.51	260.71	256.00		254.07	253.55	252.96
	260.61	266.55	258.97		256.30	253.97	253.58
	266.52	267.50	259.63		257.78	256.56	256.73
	267.13	267.76	266.00		257.79	257.37	256.85
	267.43	268.65	266.43		264.47	257.73	256.86
	268.56	269.73	266.82		265.90	264.55	264.18
	269.73	270.76	267.44		265.91	265.95	265.99
	270.35	271.49	269.15		265.93	266.12	266.06
	271.42	281.81	269.67		497.74	266.23	266.12
	281.44	342.62	270.74		503.01	318.34	373.04
	597.30	485.93	280.78		894.82	420.68	491.41
	675.85	523.92	351.01		3540.98	3563.40	3514.97
	866.89	762.66	533.48	Nb/Cu(100)	42.30	-1675.50	41.90
	3608.82	3533.35	3524.66		44.80	42.10	45.31
V/Cu(100)	47.20	-1301.35	45.07		47.95	46.45	46.93
	48.45	45.36	47.45		48.69	47.49	48.32
	49.24	47.70	47.61		49.12	48.71	51.07
	49.64	49.54	49.39		53.18	48.88	51.67
	52.36	49.62	52.79		53.73	51.58	53.73
	52.82	52.26	52.92		53.81	53.41	55.15
	54.14	53.34	53.47		54.19	54.05	56.04
	54.25	53.88	54.37		54.28	54.62	57.41
	55.37	54.29	58.21		61.52	59.68	63.10
	59.24	56.78	59.68		62.67	61.43	63.54
	63.54	61.29	62.91		63.90	64.09	64.31
	64.98	62.89	64.39		64.61	64.21	66.34
	65.04	63.39	65.79		69.65	68.57	68.16
	67.57	64.85	67.01		70.67	69.91	70.79
	71.60	68.56	71.26		72.70	70.57	72.86
	71.87	71.39	71.43		72.83	71.60	72.87
	72.55	71.63	71.47		73.20	72.43	73.74
	72.56	72.17	72.90		73.22	72.92	73.96
	74.06	72.60	74.36		73.30	73.29	74.28
	74.20	74.06	75.05		75.39	75.06	75.39
	74.23	74.10	75.50		81.22	75.65	82.44
	75.62	76.01	76.00		82.06	80.89	82.62
	83.35	76.22	82.87		84.04	83.41	84.48
	83.53	82.96	82.99		84.09	83.79	85.59
	86.69	84.09	85.72		86.26	85.98	85.70
	86.70	85.86	86.09		86.44	86.45	86.19
	86.86	86.33	86.95		88.48	86.78	87.39
	87.38	86.81	87.06		88.60	88.19	87.39

87.90	87.52	87.35	89.29	89.53	88.54
88.99	87.57	89.15	90.79	89.86	89.63
89.09	89.04	89.37	93.21	90.56	91.19
90.28	89.49	89.75	93.39	92.56	91.32
94.23	90.63	92.75	96.24	96.11	96.03
94.50	93.39	93.04	96.94	96.75	96.60
96.41	96.30	96.28	100.70	99.32	100.25
96.96	96.86	96.78	101.25	99.84	100.77
101.14	97.80	100.90	101.28	100.40	100.79
101.33	100.82	101.06	101.96	100.82	102.88
101.35	100.94	101.11	102.35	102.03	102.92
101.53	101.18	101.43	102.36	102.70	102.92
103.07	101.72	103.69	102.62	102.73	102.99
103.08	102.91	103.97	104.47	103.45	104.75
103.52	103.27	104.04	104.76	104.59	106.75
104.12	103.61	104.69	107.23	105.56	106.91
105.88	104.20	107.58	108.52	106.91	107.87
108.01	107.59	108.24	108.53	107.65	107.89
108.91	107.71	108.25	110.27	108.38	109.73
108.99	107.91	108.91	111.19	110.02	110.26
109.10	108.60	108.96	111.91	110.43	111.37
111.95	108.75	111.33	112.45	111.74	112.21
112.34	111.12	112.08	112.74	112.07	112.66
112.71	111.62	112.25	112.75	112.74	112.82
112.71	112.32	112.90	113.32	112.76	112.82
113.03	112.93	112.97	114.01	112.87	114.19
113.04	112.95	113.67	114.01	113.79	114.33
114.26	112.97	114.92	128.54	115.35	127.74
114.26	114.15	115.36	128.62	127.96	127.75
128.71	115.24	127.98	128.64	128.27	127.97
128.85	127.89	128.06	129.68	128.36	129.28
129.14	128.59	128.10	131.30	129.42	130.32
129.16	128.71	128.62	131.34	130.79	130.42
131.39	128.80	130.77	131.46	131.07	130.84
131.89	130.30	131.31	132.32	131.12	131.10
132.43	131.40	131.35	132.34	131.31	131.12
132.59	131.45	131.39	133.46	131.62	132.69
132.60	132.00	131.43	133.47	133.01	132.81
133.62	132.12	132.49	134.01	133.24	132.90
133.81	133.00	132.52	134.16	133.35	133.66
133.82	133.36	133.13	134.37	133.72	134.02
133.95	133.40	133.16	135.16	133.85	135.04
134.58	133.49	133.63	135.44	135.28	135.18
135.55	134.03	135.22	135.44	135.39	135.21

135.55	135.48	135.23	135.66	135.41	135.22
135.70	135.52	135.37	135.98	135.49	135.73
136.08	135.67	135.72	136.02	135.65	135.81
136.49	136.01	136.23	136.95	136.16	136.24
136.88	136.46	136.80	137.15	136.74	136.79
136.90	136.53	136.90	137.19	136.93	136.80
137.51	137.11	137.22	137.59	137.41	137.22
137.51	137.50	137.47	138.16	137.92	137.81
137.65	137.52	137.61	139.42	138.07	138.56
138.10	137.59	137.75	140.63	138.80	140.63
138.16	137.87	138.11	140.67	140.57	140.69
140.26	138.28	138.54	140.67	140.66	140.70
140.30	139.06	138.97	140.86	140.72	141.07
140.71	139.66	139.08	142.61	140.96	141.49
140.86	139.80	140.76	142.61	140.97	141.94
141.53	140.68	140.94	143.36	141.96	141.95
141.56	140.93	141.08	143.54	142.30	142.54
142.07	140.99	141.10	143.55	142.95	142.62
142.38	141.27	141.70	143.59	143.47	143.80
143.40	142.26	143.56	143.61	143.82	143.81
143.40	143.78	143.69	145.54	143.85	144.53
144.16	143.81	143.71	147.14	145.54	144.62
145.45	143.95	144.44	147.28	145.83	145.48
145.46	144.58	144.54	148.33	146.76	147.69
145.76	145.12	145.86	148.34	147.84	147.71
146.09	145.82	146.41	148.64	148.33	148.60
146.31	146.64	146.84	151.29	148.89	149.29
149.11	148.47	147.35	151.31	150.11	149.35
149.11	148.50	148.31	153.08	150.87	152.13
151.20	149.12	148.97	157.82	153.52	157.79
151.46	149.73	149.06	160.19	158.79	159.16
156.28	150.60	155.62	160.25	159.65	159.28
157.78	156.57	156.52	161.40	159.89	159.30
160.46	157.14	159.22	165.90	159.94	166.51
160.57	159.46	159.48	165.90	166.56	166.52
165.54	159.96	164.14	167.23	166.72	166.67
165.65	164.11	164.43	167.51	167.12	166.71
165.80	165.42	165.22	167.52	167.41	166.83
167.32	165.80	166.95	168.59	167.51	167.67
167.64	167.53	167.08	168.70	168.35	168.04
167.64	167.62	167.19	170.19	168.41	168.75
168.17	167.95	168.23	170.24	169.13	168.79
168.98	168.65	168.26	171.67	169.79	172.13
169.46	168.74	168.47	176.47	173.05	176.20

169.57	168.76	170.19	177.05	176.64	176.45
175.91	169.93	175.00	177.48	177.26	177.12
176.69	175.91	176.42	177.48	177.45	177.17
177.11	176.96	176.50	181.60	178.00	180.41
177.12	177.15	177.11	181.91	181.37	180.96
182.22	177.93	180.49	184.72	181.48	182.39
182.23	181.97	181.24	184.75	183.80	182.52
183.96	181.99	181.59	184.96	183.88	183.03
185.06	183.53	182.45	185.99	184.16	185.57
185.11	183.75	182.76	190.26	186.87	187.30
186.12	183.98	184.67	190.43	188.65	187.68
187.48	186.39	185.52	190.45	188.99	189.04
188.85	186.69	186.58	190.92	190.04	189.56
189.19	186.95	186.80	192.27	190.46	191.23
190.85	188.01	188.10	192.66	192.14	191.54
191.15	189.02	188.36	192.75	192.52	191.68
191.37	189.44	188.83	192.79	192.55	192.23
193.10	190.89	190.29	192.93	192.58	192.29
193.36	192.76	192.23	194.69	193.00	192.76
193.45	192.95	192.39	194.69	194.62	193.86
194.52	193.11	192.57	205.20	194.75	194.43
194.54	194.66	193.92	205.72	205.07	204.34
204.50	194.83	194.20	205.75	205.64	205.50
205.31	204.67	204.48	206.77	206.12	205.58
206.01	205.40	204.72	209.86	207.04	206.73
206.05	205.63	205.46	210.10	209.45	208.76
209.41	205.84	205.53	210.10	209.53	209.09
210.50	209.22	208.54	210.84	210.17	209.09
210.50	209.99	209.51	212.89	211.01	210.39
211.28	210.63	209.51	212.90	212.03	211.39
212.37	211.02	210.74	216.74	212.06	211.41
212.40	211.34	210.74	217.23	216.74	215.94
216.62	211.41	210.83	217.23	217.18	216.42
217.26	216.73	216.40	217.74	217.21	216.94
217.26	217.18	216.42	217.95	217.30	216.95
217.67	217.25	217.06	218.22	217.76	217.17
218.29	217.62	217.07	219.67	218.29	217.44
218.95	217.64	217.59	219.69	219.51	219.03
219.22	217.79	217.69	220.06	219.63	219.08
219.31	218.34	217.74	220.50	220.64	220.68
219.50	218.97	217.84	231.87	221.55	221.50
220.31	220.09	220.00	232.11	227.48	226.89
222.95	221.16	220.15	235.38	229.55	226.98
223.14	221.58	220.19	235.66	235.51	234.97

	231.36	221.65	221.29		235.67	235.59	235.08
	235.97	231.22	231.37		235.89	235.67	235.10
	235.97	235.80	235.39		237.37	235.69	235.11
	235.98	235.89	235.46		237.38	236.96	236.32
	236.71	235.98	235.48		237.60	237.02	236.33
	237.07	236.85	236.25		238.13	237.70	237.46
	237.08	236.91	236.35		238.77	238.32	237.93
	237.60	236.92	236.37		238.80	238.55	237.98
	238.36	237.96	237.77		238.87	238.77	238.03
	238.63	238.57	238.18		238.89	238.97	238.15
	238.64	238.77	238.26		245.19	239.14	238.91
	238.68	238.87	238.29		245.21	245.35	245.03
	244.45	239.10	238.40		245.21	245.53	245.43
	244.85	244.54	243.90		246.01	245.87	245.44
	244.86	244.92	244.40		246.41	246.10	245.50
	245.08	245.00	244.76		246.42	246.33	245.79
	245.69	245.02	244.77		246.44	246.44	245.91
	245.69	245.84	245.58		246.44	246.46	245.95
	246.26	246.32	245.59		249.03	246.60	246.13
	246.50	246.39	245.66		249.86	249.22	249.29
	248.59	246.80	246.57		249.88	249.38	249.32
	249.01	248.69	247.95		251.25	249.47	249.43
	249.01	248.83	248.12		251.47	251.35	250.69
	251.26	248.89	248.13		252.15	251.71	250.73
	251.29	251.44	250.96		252.15	251.92	251.28
	252.02	252.21	251.44		261.12	252.49	251.29
	252.02	252.34	251.75		261.16	261.05	260.65
	260.62	252.81	251.76		262.59	261.61	261.22
	261.46	260.82	260.29		262.62	262.39	262.27
	261.61	261.83	261.58		485.60	262.57	262.28
	261.62	261.99	261.71		3563.96	3579.31	3519.03
	488.14	262.02	261.75	Ti/Cu(110)	25.95	-1726.58	28.91
	3554.75	3567.66	3513.66		29.85	34.33	33.47
Ta/Cu(100)	47.23	-1687.70	39.36		33.54	35.61	35.94
	48.48	45.34	43.92		39.36	48.84	36.94
	50.34	48.58	49.43		47.94	49.32	49.21
	50.37	49.10	50.36		48.05	51.30	49.48
	56.66	51.03	51.93		49.54	63.64	52.49
	56.68	55.02	54.38		62.54	63.93	63.71
	57.74	56.55	56.49		63.28	65.98	64.78
	58.38	57.57	57.15		63.44	66.25	66.14
	61.65	58.53	58.90		65.67	71.73	67.46
	61.69	59.81	59.79		70.97	72.23	71.63
	64.85	61.35	61.60		71.33	72.24	72.16

65.28	63.40	63.64	72.16	72.85	72.70
72.83	65.00	64.00	72.48	77.48	72.91
75.27	69.33	70.16	77.51	78.68	77.91
75.29	72.37	71.65	77.90	79.11	77.98
76.44	74.43	75.03	78.24	80.39	78.79
77.38	75.64	77.28	78.92	82.98	80.89
77.43	76.69	77.41	82.09	84.02	82.99
77.53	77.40	77.59	83.84	88.51	84.14
77.59	77.50	78.05	90.49	90.56	90.47
81.04	77.80	78.21	90.80	93.01	91.04
81.10	78.05	79.07	91.51	93.69	93.53
84.25	79.93	80.60	93.54	94.02	95.33
84.28	82.53	82.36	94.66	97.52	95.60
86.56	83.73	83.34	95.42	98.14	96.68
87.23	85.14	85.11	97.92	98.18	98.30
90.37	86.70	86.37	98.12	99.21	99.65
90.37	87.32	88.08	98.45	100.21	101.24
93.88	89.37	88.18	105.77	105.19	105.27
94.75	90.37	92.50	106.03	107.58	106.11
95.74	92.33	92.76	108.28	108.18	107.60
95.78	94.42	93.79	108.44	108.63	108.32
96.57	94.72	94.25	108.60	109.01	108.46
96.89	95.85	95.62	109.17	109.43	109.51
97.41	96.31	96.23	109.42	109.99	109.60
103.29	97.05	96.68	110.04	110.69	110.12
104.00	97.21	97.01	110.51	110.83	110.79
104.00	100.07	102.96	110.56	111.04	111.86
104.37	102.55	102.99	113.42	113.36	113.28
104.64	103.13	103.20	113.42	114.79	114.91
104.68	104.15	103.88	114.54	115.68	114.94
104.72	104.26	104.60	115.87	116.19	115.78
104.77	104.51	104.63	115.91	116.58	116.86
105.96	104.91	104.91	116.11	120.14	117.39
105.99	105.06	104.98	119.81	120.24	118.42
106.02	105.18	105.82	120.19	120.86	118.54
109.84	105.96	105.99	127.63	128.73	127.32
112.52	106.20	106.01	128.09	128.99	128.25
113.76	107.04	109.58	129.07	129.61	128.98
113.93	109.92	112.57	130.84	130.53	130.33
113.94	112.34	112.87	133.01	134.14	133.70
113.95	113.12	113.21	133.78	134.35	133.81
115.54	113.64	113.35	134.06	135.03	134.73
115.99	114.08	113.66	135.91	135.31	135.12
115.99	114.46	114.15	136.09	136.45	136.05

126.44	115.74	115.95	136.73	137.39	136.68
126.95	116.04	116.76	137.96	137.44	137.05
126.96	116.85	126.08	138.05	137.71	137.76
127.25	126.20	126.12	138.57	139.91	139.50
128.86	126.72	126.48	140.31	140.23	140.17
131.28	127.16	128.54	140.73	141.93	140.49
132.93	128.68	130.67	141.91	143.03	142.54
133.34	131.24	131.83	143.57	144.56	143.75
133.37	132.26	131.91	143.94	145.08	144.18
133.76	132.77	131.95	144.69	145.24	145.07
133.79	132.91	132.53	146.18	146.53	146.02
133.86	133.58	133.08	146.70	147.12	147.29
134.05	133.63	133.17	147.63	149.02	147.77
135.48	133.69	133.33	149.57	150.00	149.42
135.49	133.93	134.37	149.60	150.04	149.88
135.53	135.32	134.56	149.88	151.48	149.91
135.68	135.36	134.80	151.73	152.25	150.52
136.07	135.38	135.02	152.52	152.86	152.26
136.08	135.60	135.12	154.17	155.86	155.10
136.21	135.68	135.41	155.93	156.33	155.95
136.41	135.85	135.49	156.64	157.33	156.85
137.23	135.96	135.56	157.60	158.48	157.66
137.33	136.23	136.50	158.16	158.70	159.04
137.34	136.84	136.58	160.91	161.00	160.53
138.68	136.92	136.83	164.30	165.01	163.76
138.93	137.26	137.90	164.81	165.28	164.73
139.41	138.62	138.17	169.22	169.06	168.25
140.97	138.65	138.39	173.88	173.85	172.35
140.98	139.39	140.57	175.85	175.94	173.74
141.23	140.89	140.60	176.61	176.79	175.50
141.37	140.94	140.87	177.32	177.43	175.83
141.87	141.01	141.29	179.25	179.15	176.72
141.89	141.33	141.29	179.55	180.08	178.88
143.27	141.54	141.61	179.83	180.81	180.29
143.28	141.58	142.19	182.85	183.72	180.64
144.99	143.40	143.21	183.94	184.60	183.17
145.34	143.41	143.34	184.13	184.98	184.31
145.53	143.44	143.49	185.11	185.10	184.58
145.69	145.08	143.51	185.32	185.86	184.63
145.83	145.29	144.25	185.32	186.15	185.22
149.21	145.50	144.47	185.81	187.04	185.70
149.22	146.29	147.49	186.50	188.12	185.99
149.80	148.65	147.53	187.74	188.32	187.36
149.82	149.26	149.19	188.48	188.63	187.63

152.09	149.88	149.56	188.64	188.86	187.69
152.11	150.04	149.89	191.18	192.18	188.64
154.49	151.21	149.89	191.24	193.13	192.06
158.69	151.36	153.67	193.51	193.93	192.35
158.71	154.80	157.48	196.13	196.15	192.71
159.00	158.36	157.56	196.54	196.33	194.59
163.05	158.56	158.83	197.42	197.64	195.87
165.96	159.98	160.14	201.76	201.33	196.32
166.06	161.47	164.85	203.28	205.59	200.31
168.40	164.98	164.90	210.02	210.18	203.79
169.56	166.43	167.85	211.32	211.23	208.87
169.56	168.52	168.24	211.39	211.43	209.98
169.66	168.87	168.31	211.57	211.65	210.31
169.70	169.35	168.67	211.88	211.80	211.44
169.95	169.57	168.70	212.76	213.49	212.05
172.52	169.68	168.74	213.19	213.60	212.26
172.53	169.71	171.02	213.43	214.00	212.51
176.64	172.68	171.96	214.73	214.83	213.11
178.37	173.02	175.77	215.99	216.13	214.49
178.39	176.84	177.21	218.19	217.18	215.44
180.00	178.28	177.34	219.11	219.56	215.63
180.40	178.33	179.21	219.35	220.00	218.50
181.66	180.23	179.46	220.67	220.36	219.60
181.77	180.57	179.73	221.33	221.20	219.68
183.54	181.14	179.88	221.80	222.18	220.71
187.53	181.34	181.93	222.67	222.89	221.28
187.64	183.01	185.57	224.97	223.41	221.61
187.70	187.07	186.01	227.01	227.12	223.62
189.33	187.38	187.94	228.85	228.81	226.85
190.90	188.73	189.83	231.03	231.17	228.28
192.74	190.58	190.34	232.72	233.25	230.27
193.28	192.55	191.74	233.25	233.39	232.53
193.81	193.35	192.45	233.27	233.62	232.66
193.82	193.50	192.54	233.48	233.70	233.32
194.23	193.51	192.58	235.49	234.73	233.80
194.70	194.21	192.76	239.12	238.65	234.78
195.67	194.33	193.50	239.26	239.46	238.59
196.15	194.70	193.79	239.65	239.67	238.93
196.21	196.06	194.64	240.31	239.92	239.22
205.27	196.16	198.84	240.78	240.79	239.46
205.29	205.52	205.10	242.95	242.58	240.69
206.20	205.91	205.29	243.96	244.58	241.38
206.45	206.01	205.56	429.25	249.73	244.52
210.12	206.59	206.10	489.04	379.48	366.67

210.12	209.69	208.92		893.65	406.45	497.38
210.69	210.20	208.93		3538.42	3562.63	3510.03
211.77	210.29	209.24	V/Cu(110)	23.67	-1223.44	22.48
212.72	211.86	211.07		24.34	25.08	23.89
212.74	212.08	211.61		28.12	28.67	24.07
216.54	212.30	211.62		45.75	30.36	29.71
217.25	216.59	215.60		46.89	46.28	38.59
217.26	216.77	216.31		58.23	49.39	46.63
217.43	217.07	216.35		58.81	58.55	49.61
218.02	217.34	217.15		59.03	59.25	57.90
218.38	217.91	217.50		60.44	59.62	58.64
218.46	218.46	218.05		61.55	60.83	58.88
219.54	218.58	218.19		62.17	62.24	62.19
220.63	220.35	218.80		64.15	62.42	62.36
221.63	220.49	219.75		64.63	64.63	62.65
227.98	222.82	221.22		65.45	65.61	64.38
228.18	226.61	225.05		66.45	66.62	64.81
237.31	227.51	225.11		66.52	66.72	66.65
237.32	236.93	236.20		68.59	68.34	66.83
237.87	237.04	236.21		72.20	68.37	67.53
238.21	237.70	236.61		73.46	72.29	68.92
238.72	237.86	236.93		81.92	73.94	71.43
238.73	238.45	237.47		85.38	83.62	73.17
239.32	238.50	237.48		88.61	87.52	86.30
239.55	239.03	238.16		89.20	88.25	88.20
242.99	239.23	238.57		89.65	90.58	88.97
243.00	242.30	241.15		92.29	91.38	90.56
243.67	242.43	241.19		94.09	93.88	90.79
244.42	243.72	242.79		94.97	94.94	93.03
246.13	244.35	243.40		95.22	95.30	94.06
246.13	246.07	245.90		95.23	95.54	95.35
246.53	246.13	245.94		96.11	95.93	95.78
246.90	246.20	245.98		101.46	100.84	99.83
247.49	246.63	246.13		101.46	101.30	100.06
247.53	247.41	246.30		103.25	102.07	101.26
247.88	247.61	246.34		103.35	103.11	101.55
249.10	248.00	246.86		103.59	103.14	102.13
251.66	249.26	248.15		104.12	103.67	103.09
251.74	251.54	250.89		104.20	103.74	103.27
255.56	251.70	250.91		104.31	104.51	104.36
256.47	255.18	254.32		105.49	105.96	104.46
256.47	255.84	255.15		106.00	106.07	104.83
257.07	256.31	255.19		106.50	106.63	105.81
259.80	256.74	255.55		106.82	106.64	106.40

	263.57	259.31	258.24	107.60	107.24	106.78
	263.96	263.75	263.19	108.37	107.63	106.82
	264.07	263.90	263.22	108.39	108.31	107.23
	264.16	263.94	263.43	109.24	108.82	107.49
	506.85	264.13	263.57	110.25	109.18	108.38
	3595.96	3571.55	3496.28	111.67	111.48	110.88
Zr/Cu(110)	21.87	-1532.38	19.97	113.20	112.77	111.32
	26.25	24.59	20.74	114.78	114.69	111.45
	29.34	30.76	27.45	116.49	115.53	113.80
	41.37	42.93	29.72	118.49	116.50	114.41
	42.88	43.66	43.69	118.72	117.75	116.74
	49.10	50.28	44.59	122.78	121.91	121.64
	51.59	53.92	50.07	124.65	124.46	123.83
	56.44	58.27	53.93	127.43	127.28	126.81
	58.70	59.31	59.38	128.91	128.05	126.84
	62.37	61.54	59.96	128.96	129.41	128.16
	62.79	62.78	62.18	129.27	129.50	128.55
	62.98	63.73	62.42	129.64	129.61	128.82
	64.95	64.55	63.47	129.85	129.80	128.93
	65.88	66.00	63.99	130.80	130.45	129.61
	71.46	71.99	65.76	131.88	132.44	132.19
	72.24	72.55	72.32	132.76	133.45	132.26
	73.13	73.67	72.64	133.97	134.12	133.08
	73.51	74.12	73.72	136.24	136.19	135.43
	73.58	74.15	73.74	136.34	136.86	135.66
	75.65	75.74	74.32	137.66	137.47	136.35
	79.95	84.10	75.71	137.71	137.97	137.30
	84.95	85.04	85.60	139.12	138.74	138.36
	86.37	86.50	86.02	139.39	139.34	138.49
	88.39	88.29	87.77	140.19	140.35	139.05
	88.87	88.96	88.84	140.50	140.36	139.28
	89.05	90.44	90.92	141.33	140.64	139.70
	93.40	92.88	92.45	141.60	140.78	140.08
	93.74	93.71	92.86	142.21	142.01	140.09
	94.01	93.79	93.51	142.53	142.02	141.82
	94.28	95.89	94.43	146.89	146.38	145.36
	99.26	97.72	97.39	147.01	147.10	145.39
	99.40	99.91	97.67	147.68	147.28	145.73
	99.97	99.93	99.29	148.12	148.33	146.67
	100.35	100.81	99.52	149.90	149.55	148.15
	100.79	101.10	100.82	150.92	151.43	148.32
	101.77	101.83	101.57	155.09	155.24	154.28
	102.27	101.98	101.66	156.88	157.05	156.24
	102.32	102.33	101.92	161.13	160.70	159.43

104.87	104.43	103.41	162.22	162.68	161.34
105.13	105.00	104.11	163.07	162.82	161.93
106.04	105.67	105.47	163.21	163.06	162.56
106.48	105.81	105.66	168.75	169.93	163.55
106.99	107.08	106.03	170.27	170.22	168.83
107.78	107.81	107.34	170.68	170.47	168.96
108.13	108.46	107.37	171.37	170.49	169.30
108.83	110.38	107.86	171.52	171.48	169.64
112.06	111.70	110.50	173.24	172.82	170.77
113.60	113.18	111.96	174.59	174.60	173.01
114.88	115.42	115.54	175.71	174.68	173.81
117.16	117.47	117.24	175.99	175.59	174.26
119.19	119.48	118.68	177.05	175.82	174.90
123.07	122.33	121.83	177.84	177.20	175.26
125.04	125.46	124.76	180.09	178.86	175.51
126.08	125.99	125.67	181.74	181.17	177.80
126.23	126.20	125.79	184.51	184.52	180.24
126.54	126.51	126.41	186.35	185.58	183.25
127.43	127.12	126.82	188.44	188.34	184.13
127.80	127.36	127.01	191.77	188.87	186.58
128.08	128.25	128.65	192.20	191.88	187.57
130.76	129.46	129.31	193.54	192.89	190.95
131.42	131.71	130.81	194.60	194.52	191.52
131.70	132.22	131.69	197.15	197.78	192.89
133.46	133.71	131.95	202.18	201.87	196.09
134.30	134.73	133.41	202.26	201.95	200.96
135.16	135.31	133.99	202.35	202.43	201.01
136.34	136.71	136.09	203.06	202.52	201.37
136.71	136.76	136.49	203.63	204.20	202.21
136.75	137.34	136.59	205.00	204.57	202.64
138.50	138.42	137.65	206.05	205.83	203.21
140.42	139.60	138.03	207.62	206.73	204.77
140.45	140.58	138.25	208.37	207.15	204.96
140.46	140.71	140.05	210.30	210.52	206.77
141.00	140.79	140.10	211.32	211.92	209.48
143.03	143.09	140.37	212.44	211.99	210.65
144.86	144.27	142.79	215.11	214.85	211.88
146.06	146.15	143.25	216.32	216.83	213.05
147.87	148.17	146.24	217.84	217.52	215.54
149.23	148.31	146.77	218.05	217.77	216.55
149.70	150.93	148.37	218.40	218.19	216.68
151.75	151.38	150.84	219.74	219.77	217.28
154.52	152.22	151.99	221.72	221.31	218.22
154.81	154.23	153.21	222.42	222.06	219.79

155.97	156.44	153.41		222.93	222.16	221.92
161.49	160.51	156.38		223.42	223.01	222.05
166.16	165.47	160.07		223.75	223.57	222.14
167.17	166.53	165.68		225.69	225.40	222.53
167.86	168.04	166.78		226.16	225.87	224.54
168.17	168.25	166.99		226.45	226.31	224.94
172.27	168.48	167.95		226.71	226.58	225.14
172.90	172.56	172.18		228.28	227.82	225.81
172.95	173.32	172.86		228.86	229.01	226.99
173.26	174.02	173.53		230.26	230.36	228.85
174.74	174.63	173.80		233.72	233.63	229.39
175.12	175.13	174.79		235.34	235.67	233.24
175.66	175.18	174.83		236.70	236.46	234.54
176.58	175.73	175.32		403.72	264.04	235.26
176.86	176.59	175.58		482.94	387.61	378.93
178.39	177.71	175.87		955.68	410.05	510.89
179.16	178.85	178.31		3551.13	3560.41	3505.43
180.58	179.74	178.91	Hf/Cu(110)	30.16	-2132.66	31.34
181.19	180.35	179.27		30.69	31.60	31.40
181.31	181.58	179.51		31.22	31.82	39.38
182.03	181.81	181.07		32.44	42.34	43.55
183.63	182.62	181.18		40.54	44.60	48.88
185.55	183.93	182.22		43.04	50.50	50.95
188.16	185.32	184.55		49.18	58.08	54.37
191.73	188.54	188.07		56.76	59.10	59.70
195.01	191.43	189.81		58.25	59.95	61.66
196.64	193.90	192.28		58.56	63.44	63.17
203.34	198.18	196.91		63.24	63.73	63.54
204.72	204.13	203.09		64.19	64.38	64.01
205.87	204.67	204.36		64.21	64.47	64.41
205.99	205.67	204.39		65.45	67.42	65.54
207.05	205.95	205.06		67.27	69.34	66.85
208.08	207.18	207.01		67.45	72.35	70.20
208.17	207.76	207.52		71.89	72.68	72.62
208.70	208.43	208.21		73.26	74.41	73.41
210.63	208.80	208.40		73.65	75.18	74.49
211.96	211.02	209.97		74.85	75.95	74.75
212.44	211.67	211.27		76.05	77.20	75.88
213.25	212.64	212.38		78.88	84.27	86.07
214.50	213.55	212.42		85.19	86.48	88.19
216.55	214.67	213.84		88.34	88.56	88.39
218.00	215.71	214.34		88.48	89.41	88.66
218.35	216.63	215.29		89.52	90.04	90.64
218.99	218.35	217.57		90.00	90.71	92.02

	220.53	218.50	218.40	93.06	93.95	93.02
	222.76	220.32	218.67	94.61	94.44	94.18
	223.89	222.60	220.91	95.17	95.12	94.59
	226.07	224.11	223.82	97.22	97.65	96.85
	227.71	226.34	225.28	99.35	98.73	98.99
	228.00	227.55	227.54	100.23	100.18	99.73
	228.21	227.74	227.71	100.93	100.68	99.80
	228.85	228.59	227.78	101.18	101.08	100.75
	230.07	229.04	228.30	101.36	101.48	101.13
	232.10	229.86	229.05	103.02	102.79	102.25
	233.53	231.27	231.03	103.04	103.14	103.00
	233.61	233.11	232.59	105.14	105.12	104.49
	234.39	233.90	233.87	105.53	105.40	104.51
	235.92	234.55	234.12	106.24	106.34	105.74
	236.46	235.32	235.37	106.83	106.69	105.86
	237.47	236.30	235.42	106.95	106.90	106.20
	238.59	237.82	236.49	108.43	108.83	108.19
	448.91	238.02	237.11	109.20	108.98	108.39
	486.97	376.21	328.66	110.06	110.36	109.71
	799.87	405.61	435.45	110.87	110.72	110.23
	3586.67	3553.36	3507.83	113.69	113.39	111.93
Ta/Cu(110)	22.49	-1931.92	22.61	116.40	116.65	116.54
	28.96	33.19	31.77	116.93	117.42	117.70
	31.00	33.28	32.16	118.47	118.98	118.68
	31.00	49.12	33.21	122.05	121.43	120.83
	32.77	50.57	47.79	124.80	125.46	124.90
	48.45	56.62	49.58	126.16	125.96	125.59
	51.45	61.01	53.70	126.46	126.24	125.94
	55.02	62.00	60.43	127.13	126.86	126.41
	60.15	64.37	61.26	127.83	127.49	126.90
	61.87	66.83	63.48	128.14	127.58	126.92
	64.39	67.48	65.91	128.48	128.75	129.02
	67.10	69.55	66.48	131.62	130.78	129.68
	68.34	70.13	68.46	131.83	131.82	131.75
	68.87	70.87	69.54	132.65	133.95	131.95
	71.05	73.84	70.40	133.78	133.99	133.08
	73.59	74.95	73.40	134.87	135.04	134.24
	73.96	81.19	73.75	135.32	135.11	134.63
	74.24	81.34	75.45	136.15	136.30	136.14
	80.10	82.16	81.19	136.85	137.28	136.97
	82.15	84.34	82.92	136.97	137.66	137.45
	83.28	86.78	84.45	138.83	138.88	138.49
	87.58	91.31	88.64	139.29	139.09	138.57
	89.67	92.11	91.23	140.69	140.76	139.17

91.38	92.33	92.13	140.86	140.91	140.26
92.89	96.51	92.68	141.00	141.02	140.71
96.02	96.93	94.78	142.80	143.47	143.42
96.32	98.16	97.00	146.12	146.00	144.03
98.50	100.15	97.78	146.32	146.35	146.31
100.20	101.28	98.04	146.99	147.04	146.90
100.99	102.39	99.90	149.70	150.65	150.24
101.29	104.36	102.02	150.65	150.97	150.65
104.24	104.38	103.49	151.55	152.07	152.39
106.45	107.03	104.92	155.45	155.39	154.65
106.90	107.63	106.17	156.39	155.51	155.38
107.96	107.77	107.09	157.05	157.77	157.34
108.17	107.89	107.15	161.29	160.96	160.13
109.93	111.17	108.59	166.84	167.16	164.83
111.09	111.70	111.06	167.98	167.90	166.54
112.01	112.29	111.98	169.46	169.87	167.40
112.22	113.10	112.17	169.56	169.98	169.15
113.49	113.51	112.46	171.35	171.75	169.71
113.82	114.26	113.10	173.20	173.62	171.19
114.08	115.45	113.42	173.26	174.06	173.41
115.84	116.44	115.53	173.95	174.52	174.16
116.43	116.88	115.90	174.37	174.73	174.39
117.17	117.26	115.92	175.13	175.54	174.82
117.30	117.41	116.66	176.18	175.73	175.15
119.87	119.18	117.32	176.31	176.57	175.56
120.01	120.42	120.37	177.67	177.43	176.11
122.32	122.68	121.50	177.82	178.48	176.33
131.10	131.81	130.32	178.25	178.54	178.14
134.81	134.40	134.26	178.84	179.82	178.43
135.38	135.18	134.29	181.39	182.06	179.67
135.41	135.94	134.53	181.86	182.17	181.15
135.90	136.14	135.62	181.98	182.39	181.49
136.42	136.47	135.72	183.80	182.66	181.69
136.48	136.54	135.79	186.08	186.04	182.79
136.54	136.61	136.32	188.56	189.22	185.66
137.54	138.20	137.18	191.10	190.78	188.64
137.89	138.30	138.01	193.67	192.63	189.37
139.70	138.60	138.14	198.08	200.26	191.55
143.68	143.46	141.30	203.95	204.52	199.86
143.91	144.39	141.76	204.86	205.75	203.35
144.89	144.70	143.38	205.83	205.86	204.88
145.10	144.99	143.90	206.44	206.12	205.03
146.80	146.71	146.24	206.56	206.70	205.77
146.82	146.89	146.74	207.82	208.06	206.70

148.56	148.25	147.35		208.05	208.37	207.52
150.39	150.69	149.97		208.75	208.53	207.83
150.46	150.81	150.36		211.33	211.54	208.38
150.67	150.84	150.67		211.76	211.77	210.32
150.96	151.16	150.98		212.58	212.40	210.92
151.60	151.48	151.00		213.01	213.36	212.13
151.67	152.83	151.71		214.58	214.02	212.63
153.70	154.36	152.83		214.61	215.50	213.94
153.81	154.37	153.28		215.66	215.89	214.71
155.16	154.48	153.95		218.82	218.46	215.65
156.50	156.15	154.56		219.50	218.91	217.54
157.51	156.57	155.62		220.55	220.19	218.28
158.61	157.17	156.30		223.66	222.88	218.51
162.54	163.01	156.57		223.78	223.86	222.11
165.79	165.75	161.89		226.53	226.81	223.80
168.49	168.41	165.02		228.30	228.15	225.73
168.95	168.54	166.81		228.38	228.59	227.88
175.58	175.10	167.86		228.71	228.64	228.02
175.82	175.49	174.63		229.03	229.33	228.06
175.84	175.75	174.82		229.93	229.92	228.32
177.00	176.81	174.96		232.96	232.72	229.16
179.77	179.05	175.92		233.60	233.15	232.20
180.70	180.29	179.04		233.74	234.31	233.23
180.92	180.73	179.13		234.65	234.96	234.14
182.80	183.93	180.69		236.17	236.12	234.29
184.08	184.34	183.45		236.43	236.66	236.07
184.35	185.01	184.14		236.84	237.98	236.19
184.73	185.08	184.75		238.21	238.79	238.05
187.10	187.24	185.16		471.13	278.24	238.48
187.28	187.54	185.79		525.88	403.47	338.54
187.72	187.90	186.36		757.64	449.56	490.79
188.76	187.94	186.57		3580.41	3573.08	3487.38
188.92	188.81	187.85	W/Cu(110)	21.68	-1512.88	19.26
189.39	188.90	187.94		21.82	21.62	20.63
190.74	190.83	188.53		26.19	22.48	29.18
192.69	192.72	189.82		29.13	30.55	41.67
193.65	193.11	191.93		39.64	42.79	43.27
195.32	195.29	192.71		42.50	46.60	50.25
198.34	198.04	194.63		44.73	53.84	52.51
199.81	199.27	197.13		53.05	53.94	53.91
200.55	200.57	197.77		53.80	54.79	54.53
201.11	201.45	199.46		55.53	56.30	56.29
203.96	204.78	200.69		57.68	57.91	57.87
205.65	205.11	203.70		58.65	59.05	58.98

	209.37	209.54	204.86	58.68	59.31	59.17
	209.89	210.39	208.70	58.89	59.56	59.38
	210.23	210.46	209.50	59.47	59.76	60.50
	210.31	210.65	209.89	60.57	60.23	61.07
	210.67	210.86	210.12	60.78	62.31	63.59
	212.29	212.03	210.33	61.16	64.80	65.52
	212.81	213.00	211.40	65.59	68.11	67.56
	214.67	213.53	211.82	68.28	69.06	67.91
	214.77	214.58	212.12	68.66	78.98	72.87
	217.18	216.87	213.00	79.95	83.66	80.63
	217.43	217.85	215.52	84.67	85.70	84.92
	217.62	218.47	217.42	85.01	85.84	85.48
	217.87	218.59	217.69	86.54	87.28	85.61
	218.52	219.07	218.30	86.89	89.00	85.70
	219.93	220.03	218.72	89.12	90.36	88.85
	220.48	220.33	218.81	90.15	90.53	89.17
	224.40	220.85	218.92	90.82	91.41	90.37
	224.71	224.99	222.65	91.78	91.72	90.38
	225.87	225.87	223.93	91.80	92.54	91.69
	226.15	226.43	225.58	92.36	93.58	91.85
	228.47	228.06	226.37	92.54	94.66	93.84
	231.76	231.91	227.07	94.51	95.29	94.35
	231.89	232.37	231.20	96.18	95.55	94.77
	233.66	232.66	231.75	96.53	96.54	95.87
	234.17	233.32	232.18	96.87	97.28	96.46
	235.24	233.34	232.92	97.50	97.54	96.61
	235.74	235.95	234.32	99.07	98.46	97.29
	236.68	236.78	235.56	99.16	99.38	97.86
	238.01	238.12	236.45	99.37	99.50	98.87
	239.15	238.89	237.29	100.36	100.16	99.12
	240.80	240.37	237.74	100.58	100.59	100.13
	243.04	243.33	239.24	101.58	101.53	100.93
	428.05	246.77	243.10	101.86	102.13	101.22
	498.16	391.19	335.44	103.35	102.62	101.60
	909.71	447.58	529.12	104.76	103.94	103.15
	3589.71	3571.14	3493.34	104.92	104.08	103.44
V/Cu(211)	25.90	-1886.42	26.69	105.11	108.13	103.70
	37.76	27.62	42.66	108.19	108.23	107.27
	42.53	37.54	42.91	108.89	108.30	107.61
	42.80	42.55	44.27	113.16	112.57	112.34
	44.34	42.75	49.13	115.83	115.54	114.33
	55.92	44.39	56.15	115.97	116.06	115.87
	56.65	55.60	56.43	118.76	118.65	118.40
	59.03	56.66	59.01	118.79	119.68	119.38

60.19	59.12	61.38	121.26	121.17	120.40
62.25	60.05	61.95	121.58	121.79	120.77
68.31	62.11	68.70	122.00	122.30	121.83
70.10	68.78	69.45	122.19	122.51	121.91
70.14	69.97	69.91	122.66	122.65	122.69
70.43	70.04	70.07	125.71	123.72	124.49
70.95	70.37	70.62	127.39	127.55	126.25
71.38	70.74	71.84	127.81	128.04	127.30
72.21	71.96	71.93	128.68	129.43	127.62
76.85	72.18	73.28	129.38	129.48	128.47
77.20	76.71	77.07	129.84	129.57	128.70
77.65	77.26	77.15	130.04	129.88	128.93
78.66	77.93	78.89	132.26	131.90	131.10
83.98	78.97	79.02	132.86	132.79	131.32
85.36	83.81	84.40	133.12	132.87	132.05
86.62	84.98	84.45	133.95	133.21	132.25
87.96	85.91	87.35	134.99	134.76	133.03
88.00	86.81	88.17	135.20	135.91	133.80
88.52	87.88	88.66	137.02	136.83	135.82
89.02	88.33	88.75	137.09	137.05	135.94
89.17	88.95	89.78	137.53	137.22	136.19
93.95	89.49	91.69	137.64	138.70	138.28
95.19	93.88	95.20	141.85	138.95	138.94
95.89	95.33	95.88	142.06	142.21	140.90
99.81	95.98	96.02	142.32	142.34	141.06
100.19	99.08	99.71	143.32	143.00	142.13
100.35	99.61	99.95	145.29	144.91	143.33
101.44	100.31	100.33	149.15	148.98	143.73
102.09	101.46	101.00	150.89	150.95	148.22
102.40	101.94	101.61	155.08	154.91	150.48
103.56	102.37	102.00	155.73	155.74	154.22
103.75	103.28	103.19	156.16	156.45	155.14
104.83	103.37	103.42	156.43	156.58	155.40
105.56	104.77	104.35	164.08	163.78	156.51
105.72	105.51	105.24	164.32	164.24	164.17
105.81	105.53	105.74	165.02	165.00	164.18
106.80	105.74	106.26	166.07	165.55	164.82
107.40	106.77	106.98	166.59	166.41	165.23
107.58	107.60	107.72	167.50	167.40	166.18
108.72	107.83	107.76	168.13	168.13	166.76
109.03	108.51	109.03	170.10	170.21	167.47
109.07	109.19	109.72	171.60	170.62	169.21
110.24	109.30	110.43	171.66	171.44	170.12
111.47	110.42	111.04	171.85	171.74	170.35

117.78	117.52	117.76	171.94	172.00	171.04
117.88	118.22	118.50	176.52	176.15	171.39
119.76	120.20	120.71	178.02	176.91	175.93
119.96	120.23	120.74	179.81	179.65	177.08
122.06	121.81	122.40	182.15	181.49	178.74
122.34	122.51	122.99	182.34	182.05	180.30
123.11	123.09	123.55	187.25	186.82	181.34
123.25	123.53	124.34	187.29	187.42	185.64
123.73	123.90	124.71	193.03	193.14	186.20
124.69	124.17	124.88	196.03	196.06	192.08
125.50	125.70	125.80	196.86	196.87	195.52
125.85	125.91	125.91	196.87	196.92	195.93
127.89	127.74	127.27	197.78	198.01	196.83
128.82	129.21	128.96	199.26	199.11	197.37
129.40	129.30	129.07	200.04	199.70	197.93
129.78	129.49	129.36	201.11	201.15	199.58
130.20	129.77	130.15	201.29	201.51	200.15
131.26	131.23	131.24	202.70	203.17	200.59
132.39	131.90	132.18	202.70	203.62	201.60
134.18	134.12	133.72	204.58	204.11	203.59
134.24	134.29	134.26	205.44	205.41	204.07
134.58	134.42	134.36	206.19	205.63	204.28
134.71	134.58	134.47	211.34	210.97	204.35
134.79	134.69	134.81	212.62	212.79	209.80
135.08	134.88	135.93	212.91	213.42	211.99
136.02	135.80	137.18	213.36	213.44	212.31
138.00	137.81	138.77	213.94	214.16	213.23
139.72	139.56	138.97	216.33	214.39	213.42
139.92	140.06	140.06	217.84	216.24	215.59
140.33	140.35	140.10	218.95	217.28	216.47
140.43	140.40	140.44	219.44	218.92	218.27
140.94	140.99	140.59	219.94	219.30	218.40
141.35	141.22	141.11	220.13	220.19	218.42
143.22	143.05	143.50	221.00	220.32	219.16
143.93	144.08	143.77	221.31	221.21	220.13
144.03	144.19	144.00	221.51	221.96	220.69
144.41	144.52	144.53	222.34	222.11	221.03
144.53	144.79	144.70	223.04	223.26	221.78
145.95	145.89	146.02	224.98	225.76	222.58
147.13	147.27	147.01	226.68	225.93	224.87
149.00	148.86	148.72	226.69	226.50	225.58
149.21	149.18	149.31	229.74	230.06	226.23
149.68	150.20	149.83	233.60	234.02	228.91
152.00	152.21	152.03	414.80	244.78	233.59

152.05	152.38	152.31		505.15	395.79	361.51
153.25	153.03	152.56		913.77	526.99	536.61
153.54	153.54	153.07		3605.67	3571.59	3508.01
154.11	153.66	153.87	Zr/Cu(211)	23.63	-1737.38	22.47
156.46	156.31	156.39		44.51	24.17	23.21
157.40	157.34	157.26		44.59	25.95	36.42
158.52	158.61	157.66		48.96	44.15	43.46
159.14	159.00	157.92		49.48	44.30	43.83
159.31	159.09	158.82		50.28	49.32	49.21
159.37	159.40	159.40		51.03	50.57	50.27
159.58	159.61	159.46		58.51	51.04	50.90
160.56	161.66	160.93		58.74	58.50	57.46
161.70	161.92	161.59		60.11	59.11	59.51
162.15	161.93	162.12		66.57	60.68	61.15
162.75	162.83	162.50		68.89	67.64	66.56
162.95	163.47	162.82		70.50	68.83	68.82
163.88	163.54	163.10		71.77	71.06	69.54
164.06	164.36	163.46		71.91	71.73	70.00
164.38	164.54	164.50		73.07	71.91	72.02
165.20	165.29	164.60		76.02	73.37	72.43
166.83	166.89	165.58		77.19	75.61	73.97
167.49	167.05	166.45		78.06	77.56	77.41
168.03	167.88	167.47		78.76	78.56	79.05
168.34	168.12	167.69		79.52	79.44	79.94
171.44	171.32	168.95		82.32	79.84	80.01
171.69	171.59	170.71		84.49	81.88	80.75
171.87	171.77	171.37		84.72	84.97	84.66
172.21	172.45	171.97		85.82	85.12	85.48
172.98	173.09	172.60		86.67	85.76	85.64
173.51	173.25	172.73		87.78	88.04	87.51
173.61	173.43	172.95		88.12	88.67	88.84
173.77	173.83	173.00		88.78	88.94	89.61
175.08	174.27	173.65		91.25	91.67	91.68
175.66	174.94	173.99		91.84	92.07	92.22
179.86	179.58	175.06		92.32	94.00	93.75
184.00	183.99	180.16		92.66	94.65	95.92
184.65	184.16	184.39		96.52	96.48	96.32
186.54	186.24	184.70		97.23	97.65	97.30
186.76	186.54	185.76		97.52	97.67	97.55
188.49	187.33	186.03		98.11	98.25	98.55
188.94	188.53	186.47		100.05	99.69	98.81
189.38	188.75	188.32		100.70	100.75	99.25
189.62	189.82	188.41		101.26	101.24	100.27
190.10	189.92	189.11		101.40	101.50	100.79

190.70	190.21	189.80	101.79	102.45	101.00
192.48	192.10	189.83	103.04	103.11	102.60
193.55	193.49	191.78	103.39	103.64	102.77
194.66	194.31	193.35	104.85	104.73	103.65
196.28	195.75	193.87	105.05	105.66	104.33
196.83	196.26	195.55	107.37	106.99	105.96
196.87	196.50	195.58	108.68	108.66	107.00
197.80	197.21	196.09	109.25	109.39	108.07
198.19	197.75	196.89	109.79	109.53	109.29
199.63	199.55	197.67	110.93	111.60	109.50
200.94	200.84	199.16	115.21	115.46	111.78
201.28	200.95	200.48	115.63	116.14	115.04
202.94	202.92	200.57	116.36	117.34	115.56
203.58	203.09	201.94	117.42	117.36	116.97
204.96	204.15	202.67	118.12	118.34	117.23
205.31	204.49	204.12	118.13	118.42	118.16
205.63	205.19	204.21	120.37	121.01	118.27
206.96	206.32	204.73	121.04	121.52	120.71
209.99	209.82	206.17	121.40	121.69	120.76
211.18	210.86	209.81	123.08	123.04	121.22
212.55	211.11	210.89	123.14	123.30	122.38
212.86	212.30	211.31	123.73	124.19	123.02
213.77	212.82	211.66	125.78	125.75	124.09
215.73	215.53	212.82	127.55	128.04	125.14
216.18	215.89	215.52	128.63	129.03	127.89
217.09	216.27	216.10	128.71	129.10	127.95
220.16	218.09	216.29	129.39	129.28	128.96
221.33	220.17	219.95	130.22	130.37	129.35
221.92	221.27	221.03	130.23	130.68	129.92
225.54	221.77	221.54	130.97	130.90	130.25
226.41	225.34	225.23	131.37	131.59	130.29
240.32	226.32	226.04	132.56	132.87	131.11
242.48	240.73	241.13	132.72	133.15	132.38
244.78	241.45	241.84	134.00	133.76	132.76
246.09	244.78	245.24	134.49	134.45	133.66
247.75	245.56	245.33	134.53	134.98	134.31
247.89	247.86	247.17	134.98	135.10	134.79
248.91	247.98	247.85	135.35	135.36	135.02
252.05	248.89	249.30	136.35	136.30	135.68
253.14	251.80	251.20	136.68	137.45	136.09
255.52	253.11	252.60	137.85	138.62	137.26
256.30	255.33	254.54	140.01	140.05	139.00
258.10	256.09	255.45	140.04	140.49	139.45
258.48	258.13	256.89	141.42	141.30	140.10

	259.36	258.73	257.47	141.82	141.69	140.78
	260.92	259.20	258.27	141.83	142.01	141.34
	261.33	260.57	259.92	142.09	142.01	141.44
	264.30	261.21	260.31	143.34	143.70	141.84
	266.51	264.25	262.83	144.15	143.87	142.58
	267.88	266.47	265.32	144.19	144.88	142.72
	269.42	267.81	266.93	145.79	145.85	145.24
	521.08	269.43	268.69	146.25	146.77	145.63
	532.55	412.27	370.14	146.76	147.03	146.45
	959.93	423.86	493.96	147.80	148.10	146.74
	3558.02	3567.68	3540.18	148.75	148.38	147.42
Nb/Cu(211)	26.66	-1468.84	25.44	148.88	149.30	148.34
	37.93	27.07	41.87	150.40	150.51	149.01
	41.83	41.27	42.38	150.94	151.27	150.52
	42.25	41.99	44.21	151.86	152.25	150.72
	44.64	42.19	54.46	153.15	152.50	151.95
	54.43	44.74	56.00	153.33	153.39	152.21
	56.75	54.01	56.73	154.19	154.20	153.40
	58.74	56.72	59.53	154.76	154.94	153.50
	59.78	58.68	60.11	155.36	155.18	154.21
	62.29	59.41	63.13	155.92	156.33	154.28
	68.27	62.07	67.25	156.84	156.68	155.22
	69.66	68.41	69.63	157.49	157.17	155.41
	70.10	69.56	69.73	158.07	158.20	156.51
	70.12	69.61	69.98	158.74	158.83	157.70
	70.29	70.04	70.32	159.29	158.87	158.19
	71.30	70.56	71.68	159.40	161.17	158.40
	72.01	71.05	71.95	162.25	162.70	161.13
	77.08	71.74	73.32	163.45	163.06	162.58
	77.42	76.47	76.66	163.53	163.77	162.62
	78.03	77.28	77.23	164.43	164.19	163.42
	78.46	78.07	77.77	166.05	166.03	163.68
	82.60	78.36	79.09	166.12	166.40	165.44
	83.01	82.45	83.73	166.41	166.52	166.20
	85.04	84.74	84.25	167.47	168.60	166.53
	85.20	84.80	85.54	170.74	170.95	167.99
	86.49	86.02	86.80	172.09	171.43	169.90
	87.99	87.79	87.67	172.92	173.21	171.04
	88.34	88.66	88.49	174.74	175.12	173.00
	88.79	88.81	89.19	174.85	175.47	174.31
	89.47	89.56	89.74	175.41	175.60	175.25
	93.47	93.76	95.21	176.83	177.53	175.56
	95.43	95.77	95.67	177.31	177.92	177.50
	96.01	96.18	95.90	178.87	179.52	177.72

98.17	96.78	97.49	180.12	180.84	179.56
99.94	99.83	99.63	180.84	180.95	179.91
100.02	100.08	99.88	181.92	182.57	181.22
101.38	101.07	100.86	183.61	183.70	182.48
101.78	101.65	101.15	183.81	184.07	183.17
102.29	102.28	101.84	187.17	187.40	183.71
102.91	102.70	102.30	187.89	187.75	186.82
103.89	103.44	103.31	187.94	187.88	187.65
103.94	103.80	103.75	189.34	189.58	187.68
105.39	105.07	104.82	190.08	190.58	189.48
105.80	105.60	105.12	192.55	192.44	190.39
106.45	105.74	106.00	193.87	193.83	192.18
107.53	107.27	107.15	197.24	197.24	193.47
107.86	107.64	107.60	198.78	199.03	197.16
107.89	107.96	107.62	198.85	199.06	198.47
108.68	108.08	108.45	199.65	199.70	198.57
108.88	108.83	108.87	200.39	200.40	199.14
109.10	109.34	109.94	201.13	201.51	199.70
110.69	110.81	110.83	201.76	202.02	201.24
117.89	117.98	118.21	201.94	202.03	201.54
118.35	118.05	118.40	203.05	202.98	202.03
119.26	119.36	120.51	203.58	203.40	202.55
120.56	120.49	120.70	204.75	204.62	202.75
121.33	121.29	121.50	208.32	208.12	203.75
122.06	121.38	122.38	208.50	208.66	206.82
122.89	122.75	122.41	209.63	209.61	208.24
123.30	123.14	123.19	210.46	210.88	208.68
124.02	124.28	123.80	212.94	212.61	210.71
124.87	124.85	124.85	213.03	213.08	211.91
126.41	125.79	125.50	214.73	213.89	212.06
126.81	126.44	126.32	215.25	215.33	213.07
128.01	127.76	126.45	215.99	216.08	214.97
128.14	128.45	127.11	216.42	216.32	215.58
129.51	129.42	128.58	220.11	220.16	215.66
129.70	129.48	128.90	220.67	220.68	219.87
130.30	129.75	129.54	221.22	221.22	220.41
131.16	130.97	130.04	224.44	224.75	220.70
132.81	132.45	131.15	227.78	228.14	224.44
133.43	132.63	132.51	228.81	229.26	227.76
134.03	133.88	132.71	228.95	229.87	228.95
134.13	134.00	133.58	229.87	230.03	229.50
134.66	134.56	134.24	234.33	235.83	229.85
134.92	134.76	134.38	235.91	236.07	234.87
135.36	134.76	134.51	237.13	236.83	235.72

136.35	135.43	135.02		239.60	239.46	236.90
138.34	138.44	135.94		239.98	239.58	238.16
139.88	139.82	138.60		241.29	240.85	238.20
140.21	139.88	139.13		241.37	241.13	239.72
140.31	140.20	139.81		243.33	243.10	240.19
140.53	140.55	140.29		243.77	243.20	242.10
140.92	140.93	140.52		244.11	243.97	242.21
141.49	141.04	140.85		245.03	244.82	242.96
143.41	143.28	140.94		245.91	245.07	243.72
144.15	143.83	143.46		245.93	245.73	244.58
144.21	144.09	143.86		247.08	246.62	244.90
144.41	144.50	143.93		248.08	248.01	245.66
146.89	145.46	144.91		248.45	248.50	247.40
146.99	146.74	146.43		249.18	248.72	247.96
147.34	147.18	146.60		250.32	250.29	248.31
149.46	149.41	146.62		252.43	251.14	249.63
149.65	149.80	149.08		255.21	252.43	251.27
150.71	150.42	149.66		256.82	255.25	252.41
151.92	151.80	149.89		485.19	257.19	254.57
152.14	152.30	151.86		565.38	357.74	323.35
154.49	153.45	152.38		797.32	431.39	517.46
154.53	154.17	152.96		3534.58	3570.35	3513.91
155.91	155.47	154.10	Hf/Cu(211)	20.99	-1674.29	23.91
156.97	156.71	155.06		40.37	22.98	42.67
157.39	156.87	156.31		43.70	42.32	42.89
158.18	157.98	157.15		45.88	43.58	44.61
159.28	159.19	157.19		48.14	47.49	47.66
159.58	159.27	158.64		49.70	48.94	49.12
160.18	160.07	159.07		52.83	50.89	49.29
160.32	160.51	160.14		59.19	57.17	52.86
161.79	161.85	160.78		60.12	59.81	59.17
162.50	162.06	161.55		61.75	60.73	59.47
162.72	162.56	162.45		65.70	64.57	62.15
163.63	163.17	162.49		68.53	67.82	66.74
163.80	163.63	163.09		70.16	69.00	68.86
164.35	164.26	163.45		70.74	70.20	69.61
164.56	164.60	163.73		71.61	71.36	70.74
165.75	165.11	164.43		74.34	71.79	71.25
166.10	166.10	165.18		75.51	74.29	71.99
167.29	167.15	165.77		77.39	76.22	74.40
168.11	167.76	166.68		78.62	78.13	76.55
168.54	167.99	167.42		79.17	79.42	78.61
170.25	170.07	167.65		80.83	79.55	79.81
171.39	170.95	170.08		82.85	81.29	80.19

171.76	171.42	170.59	84.90	83.89	81.12
173.02	172.48	170.73	85.64	85.20	84.47
173.16	172.55	172.15	86.74	85.98	84.96
173.35	173.01	172.51	87.82	87.95	86.05
173.61	173.13	172.76	88.39	88.19	87.79
174.19	174.18	172.81	88.76	89.07	89.06
175.38	174.30	173.99	89.63	89.57	89.43
175.39	174.86	174.64	90.32	90.63	90.59
176.08	176.04	174.97	91.89	92.32	92.41
180.62	180.14	175.58	92.52	94.42	92.54
185.43	182.64	180.30	96.20	96.31	95.89
186.27	185.54	185.08	97.25	97.35	96.33
186.30	185.79	185.35	97.62	98.10	97.36
187.93	185.86	185.52	97.89	98.42	98.42
188.54	187.30	186.60	99.87	99.77	99.24
188.97	188.28	187.41	99.93	100.03	99.45
189.37	188.93	187.95	100.37	100.85	100.11
190.23	189.13	188.80	100.78	101.06	100.99
191.29	189.85	189.64	101.71	102.47	101.42
192.17	191.49	190.21	102.75	102.70	102.87
193.60	191.88	190.52	103.01	103.46	103.36
194.10	193.17	192.93	104.31	103.92	103.62
195.49	194.45	193.23	104.63	104.49	104.18
196.39	194.80	194.36	105.30	106.38	106.02
197.08	195.80	195.71	107.32	107.65	107.91
197.55	196.74	196.07	108.76	108.75	107.97
197.70	196.80	196.22	109.41	109.30	109.54
199.24	197.74	197.04	109.75	109.62	109.82
200.37	198.45	198.18	110.94	111.28	111.31
201.19	199.89	199.77	114.61	115.61	115.14
201.96	201.13	200.53	115.32	115.83	115.45
204.10	201.48	201.05	115.77	116.26	116.29
204.79	203.00	202.29	117.58	117.69	117.44
205.09	203.75	203.96	117.85	118.10	117.81
205.78	204.90	203.97	117.93	118.17	118.01
207.25	205.74	204.86	119.68	120.10	119.88
208.02	206.14	205.55	120.45	120.68	120.51
210.09	207.36	206.71	120.63	121.18	120.79
212.08	209.88	209.79	122.82	122.71	122.58
212.96	210.71	211.13	122.89	123.17	123.09
214.09	211.80	211.55	123.69	123.64	123.62
215.92	213.37	211.73	125.92	125.96	125.40
215.98	214.89	215.18	127.15	127.68	127.77
216.06	215.86	215.54	128.41	128.92	128.42

	217.25	216.05	215.83	128.59	129.09	129.11
	220.53	216.12	216.25	129.22	129.42	129.34
	221.63	220.37	220.56	129.77	129.73	129.57
	222.82	221.33	221.30	130.09	130.62	130.20
	226.39	222.01	222.14	130.36	130.79	130.79
	226.41	226.05	225.75	131.07	131.23	130.96
	243.21	226.10	226.26	132.54	132.74	132.40
	244.49	243.04	242.70	132.67	132.93	132.94
	246.74	244.13	243.57	133.57	133.75	133.70
	247.38	246.56	246.47	134.23	134.86	134.89
	248.74	247.15	246.60	134.76	135.00	135.07
	250.76	248.53	247.53	134.94	135.08	135.09
	251.84	250.18	249.40	135.34	135.16	135.55
	253.52	251.25	251.73	135.56	136.35	136.25
	255.12	253.34	253.35	136.51	136.40	136.48
	256.26	254.71	253.81	137.04	137.92	138.32
	256.42	255.06	254.50	139.80	139.83	139.44
	258.13	256.13	256.54	140.10	139.97	139.52
	258.19	257.54	256.61	140.41	140.74	140.55
	259.35	258.06	256.84	141.41	141.44	140.89
	260.81	258.65	257.88	141.53	141.56	141.19
	260.94	260.30	259.84	142.35	141.73	141.70
	263.86	260.46	260.02	142.95	143.02	142.45
	266.12	263.55	261.40	143.47	144.10	143.57
	267.70	265.87	264.72	144.31	144.61	145.11
	269.17	267.31	266.47	145.79	145.79	145.54
	530.93	268.97	268.49	146.10	145.91	146.05
	545.92	392.51	341.57	146.73	147.02	146.83
	876.07	411.02	477.52	148.03	147.46	146.91
	3573.99	3573.69	3534.27	148.04	148.64	148.75
Ta/Cu(211)	22.34	-1384.83	24.37	148.66	148.79	149.12
	36.69	22.32	36.67	150.33	150.59	150.59
	45.95	35.15	46.15	150.88	151.08	150.76
	47.22	45.89	47.10	151.75	152.15	152.18
	52.86	47.26	53.07	152.56	152.81	152.34
	58.49	51.58	58.94	153.10	152.96	153.09
	59.57	57.55	59.51	153.87	153.38	153.16
	61.87	59.79	61.78	153.91	154.07	153.80
	62.12	61.70	62.34	154.60	155.01	154.40
	62.21	61.96	62.50	155.67	156.10	155.46
	62.91	62.13	64.16	156.41	156.14	155.48
	64.59	64.71	67.74	156.85	156.75	155.88
	68.04	67.18	69.20	158.02	157.81	156.75
	69.42	69.47	70.30	158.61	158.75	157.62

70.18	69.89	71.11	158.82	159.86	158.59
71.62	71.12	71.62	160.25	160.22	159.48
73.27	72.70	73.26	161.78	162.41	160.19
74.11	73.27	74.72	162.90	162.85	162.52
74.71	74.43	76.46	163.17	163.32	162.76
76.52	76.42	78.68	164.28	163.96	163.18
79.44	79.14	79.97	164.80	165.23	163.74
81.09	80.73	80.42	165.05	165.42	164.91
83.11	83.00	82.95	166.52	166.52	165.19
84.59	84.20	83.82	166.79	167.44	166.40
85.56	85.42	84.90	169.08	168.66	167.49
87.23	87.05	86.04	171.01	171.29	168.10
89.46	88.62	87.24	172.91	173.31	171.69
89.79	90.01	90.03	173.54	174.03	172.80
91.48	90.67	90.55	175.33	175.48	174.35
91.56	91.53	91.17	176.33	176.16	175.08
92.48	92.86	91.66	176.84	177.45	175.86
93.90	93.03	93.22	176.94	177.61	177.45
94.58	93.50	94.03	179.01	179.35	177.85
99.71	99.67	97.27	179.19	179.98	179.37
101.08	99.90	99.22	181.52	182.04	180.42
102.39	102.05	100.89	181.98	182.15	181.21
103.54	102.36	102.25	183.56	183.30	182.14
103.71	103.02	103.05	184.20	184.76	182.83
104.04	103.16	103.33	186.51	186.90	184.78
105.26	104.64	103.76	187.23	187.29	186.77
105.93	105.17	104.60	187.56	187.41	187.06
106.21	106.03	105.08	189.06	189.38	187.27
106.56	106.18	105.34	189.58	190.07	189.34
106.93	106.83	106.66	191.98	192.01	190.03
107.40	107.09	107.26	193.71	193.49	191.86
108.09	107.53	107.45	196.70	196.74	193.16
109.15	108.36	107.49	198.69	198.80	196.70
109.88	109.27	109.15	199.28	199.11	198.61
110.98	110.06	110.16	199.42	199.79	198.62
111.91	110.72	111.12	199.98	199.83	199.27
112.74	111.98	111.61	200.58	200.82	199.59
119.38	112.17	112.00	201.62	201.87	200.62
119.47	118.60	117.80	201.65	202.14	201.64
121.78	119.23	118.99	203.16	202.67	202.02
122.04	122.36	122.79	203.24	202.96	202.41
122.45	122.48	123.23	203.77	203.91	202.50
122.92	123.12	123.40	205.86	205.06	203.46
123.22	123.17	123.53	209.25	208.99	203.61

123.80	124.28	124.81		209.83	209.55	208.71
126.03	124.64	124.98		210.16	210.23	208.72
126.97	126.36	126.51		212.27	211.45	209.97
127.56	126.94	126.72		212.64	211.69	210.86
128.03	127.12	127.27		213.27	213.18	211.05
128.52	128.25	128.00		214.61	214.76	212.74
129.87	128.87	128.60		216.00	215.90	214.95
130.10	129.51	129.04		217.31	216.71	215.56
130.62	129.71	129.44		220.15	219.81	216.03
130.84	130.22	129.68		221.12	220.78	219.76
131.91	130.72	129.92		221.17	220.85	220.48
132.99	131.49	131.07		224.51	224.82	220.58
133.25	133.36	132.90		228.35	228.69	224.72
134.17	133.42	133.11		228.53	228.88	228.55
134.70	133.99	133.80		229.54	229.89	228.81
134.86	134.65	134.30		230.01	230.01	229.47
135.63	134.70	134.69		236.24	235.72	229.96
137.20	135.39	134.97		237.15	236.63	234.93
137.73	137.41	136.13		240.03	239.50	235.99
138.27	137.76	137.56		240.97	240.25	238.29
139.49	138.23	138.01		241.07	240.54	239.37
140.02	139.45	139.06		241.57	241.36	239.74
141.01	140.04	139.49		242.06	241.74	240.72
141.15	140.81	139.92		243.46	243.19	241.42
141.69	141.26	140.73		243.87	243.69	242.63
141.87	141.57	141.42		244.50	244.05	242.88
141.91	141.58	141.56		245.43	244.78	243.92
143.01	142.28	142.05		246.43	245.48	244.56
143.64	143.28	142.65		246.51	246.01	244.75
145.52	143.85	142.92		246.93	246.59	244.96
146.07	145.07	143.91		247.76	247.73	246.02
146.90	145.76	145.19		248.01	248.09	246.37
147.24	146.71	145.80		248.47	248.39	247.64
147.66	146.96	146.20		250.64	250.62	248.41
150.32	147.71	147.59		251.66	251.23	250.36
150.98	150.37	147.86		252.18	251.89	250.74
151.50	150.78	149.93		255.50	255.38	251.09
152.72	151.71	150.39		548.61	317.33	254.64
153.21	152.69	151.68		584.45	393.33	340.47
154.24	153.17	152.37		778.55	470.46	494.98
154.31	153.77	152.40		3566.57	3571.27	3498.48
155.75	154.26	152.89	W/Cu(211)	23.55	-1224.30	23.95
157.23	155.12	153.85		40.72	26.28	40.73
157.52	155.56	154.29		41.55	40.82	43.44

157.98	157.00	155.38	45.83	42.91	45.78
158.05	158.17	157.03	50.05	45.94	51.00
158.98	158.33	157.77	53.94	46.39	53.37
159.32	158.37	158.32	56.93	50.87	58.68
160.23	159.09	158.49	59.18	54.09	58.94
161.18	160.15	158.86	61.61	57.05	61.22
161.35	160.89	160.65	67.82	59.24	66.58
162.53	161.25	160.95	68.99	62.21	67.27
162.71	162.48	161.30	70.35	68.02	69.63
163.94	162.56	162.29	70.51	69.11	69.69
165.43	163.91	162.50	71.12	69.68	70.97
167.49	164.87	163.46	71.43	70.84	72.36
167.72	167.60	164.93	75.91	71.15	73.80
167.97	167.62	167.26	77.51	71.73	74.15
168.26	167.94	167.45	79.10	75.04	77.63
168.66	168.42	167.83	79.95	77.75	78.23
169.13	168.78	168.24	80.00	79.30	79.52
169.86	168.82	168.36	82.75	80.43	80.25
170.19	169.13	168.54	84.83	80.62	81.76
170.51	169.62	169.09	84.93	82.82	83.82
171.27	169.99	169.56	86.02	84.92	84.97
172.19	171.05	169.74	87.04	85.00	86.70
172.88	172.04	170.74	88.08	87.53	87.31
175.14	172.80	171.49	88.11	88.53	88.00
175.17	175.09	172.90	89.14	88.61	88.53
176.26	175.21	173.65	89.30	89.17	88.86
179.30	175.95	174.57	92.19	89.39	89.25
181.92	179.81	175.09	93.10	92.65	92.27
181.99	182.10	180.51	95.55	93.33	93.37
188.52	183.03	182.05	99.07	95.10	96.28
188.96	188.52	183.23	99.59	95.68	98.11
189.57	188.84	188.28	100.74	99.48	99.04
191.69	189.11	188.37	100.89	99.73	99.62
192.16	191.25	188.64	101.35	100.81	100.52
192.65	191.87	190.92	101.77	100.94	100.68
193.40	192.14	191.23	103.13	101.50	101.89
194.69	193.34	191.56	103.45	102.03	102.10
195.08	194.00	193.14	104.28	102.82	102.78
195.37	194.76	193.76	105.16	103.81	104.36
195.66	195.37	194.33	105.91	104.44	104.66
197.19	195.92	195.13	106.32	104.89	105.76
197.49	196.94	195.57	106.47	106.32	106.39
198.25	197.11	196.81	107.31	106.53	106.94
200.72	198.10	197.08	107.59	106.76	106.96

201.53	200.80	197.39	108.81	107.08	107.99
203.76	201.24	199.90	109.37	107.91	108.78
203.87	203.28	200.79	111.10	109.22	109.45
205.70	204.40	202.06	111.19	109.75	111.60
206.51	204.87	202.38	116.20	111.51	111.84
207.21	205.26	204.00	117.52	111.74	116.88
209.36	206.79	204.41	118.70	117.49	117.56
209.57	209.38	206.13	120.00	117.97	118.94
209.66	209.85	209.04	121.60	120.47	119.65
210.19	209.97	209.79	122.46	121.67	121.40
211.31	210.46	209.88	122.88	122.73	122.23
213.01	211.12	210.47	123.42	123.28	122.37
214.31	212.78	211.07	123.68	123.44	123.06
214.59	214.06	212.50	123.87	123.59	123.31
215.25	214.19	213.83	123.97	123.86	123.60
215.59	215.15	213.98	124.06	123.89	124.29
216.09	215.88	214.42	125.01	124.83	125.35
216.35	216.50	215.25	125.79	125.61	125.88
217.44	217.16	216.50	126.15	125.83	126.34
218.71	217.46	216.94	128.33	126.51	126.60
220.21	218.68	217.36	129.08	126.93	126.83
223.68	219.41	218.56	129.25	128.99	128.41
225.88	225.58	219.00	129.90	129.42	129.77
226.39	225.75	225.22	131.03	130.12	129.89
234.03	232.40	225.27	131.42	130.22	130.16
239.96	239.69	232.33	132.05	131.32	130.52
240.21	239.86	239.31	132.83	131.73	131.29
244.41	243.93	239.43	133.66	131.93	132.11
244.94	244.59	243.40	134.07	133.20	132.50
246.36	246.04	244.55	135.21	133.79	133.03
246.73	246.51	245.05	135.59	135.07	135.09
248.50	248.33	246.27	135.75	135.57	135.22
248.82	248.37	247.91	138.13	135.61	135.61
250.29	250.35	248.04	138.78	138.13	137.97
251.41	250.65	249.80	141.12	138.63	138.59
251.51	251.38	250.03	141.23	140.97	140.63
252.08	251.67	250.75	141.58	141.28	141.06
252.37	252.24	251.05	142.38	141.89	141.79
253.51	252.85	252.05	143.78	142.59	142.56
254.53	254.14	252.66	144.77	144.04	143.43
255.82	254.44	254.34	145.81	145.19	144.26
256.08	255.92	255.50	147.46	145.50	144.88
258.25	257.92	255.59	147.71	147.76	148.03
260.54	260.35	257.69	148.86	148.02	148.08

	262.25	262.07	260.07	148.89	148.71	148.48
	600.80	262.24	262.04	149.29	148.97	148.58
	619.16	431.65	330.40	150.36	149.66	149.50
	881.62	453.20	491.55	152.28	150.32	149.62
	3602.16	3574.90	3517.56	152.55	152.03	150.23
Sc/Cu(320)	7.50	-1371.09	6.75	153.39	152.10	150.45
	10.36	7.80	10.57	153.42	153.06	151.60
	12.51	12.00	13.49	154.53	153.39	152.17
	28.41	17.80	16.27	154.95	154.35	153.68
	28.92	26.62	27.15	155.85	154.60	153.90
	29.26	28.43	28.69	156.11	155.94	154.98
	35.60	29.15	30.07	156.58	156.19	155.62
	38.70	35.50	35.64	157.92	156.52	156.03
	40.52	38.50	38.46	159.00	157.56	156.90
	42.44	40.81	40.75	160.05	158.86	157.84
	51.53	42.28	41.96	160.22	159.82	159.06
	53.51	50.83	47.44	160.38	160.08	159.50
	55.42	53.44	52.75	160.66	160.50	159.77
	56.84	55.77	53.92	161.62	160.87	160.75
	58.08	57.41	57.51	162.08	161.63	160.96
	61.16	58.58	58.06	162.62	161.97	160.98
	62.47	60.02	59.36	163.25	162.44	161.46
	62.98	61.90	61.56	166.20	163.50	163.05
	63.22	62.69	62.84	166.63	166.36	166.41
	63.46	63.13	63.22	167.29	166.70	166.61
	63.94	63.50	63.46	167.51	167.20	166.72
	64.58	63.69	63.87	168.40	167.23	166.94
	65.36	64.07	64.15	168.65	168.33	167.94
	65.49	64.72	64.54	170.08	168.58	168.07
	65.86	65.68	65.31	170.25	170.15	169.55
	66.46	66.00	65.44	170.67	170.25	169.95
	68.63	66.38	66.32	171.95	170.91	171.15
	69.12	68.30	67.54	172.09	171.94	171.71
	69.55	69.28	68.66	172.32	172.21	172.08
	69.66	69.29	69.07	173.51	173.37	172.93
	71.11	69.77	69.56	174.44	173.86	172.96
	72.11	70.83	70.61	175.17	174.69	174.36
	72.66	71.55	71.48	175.39	175.35	175.02
	73.24	72.78	72.34	177.99	175.64	175.48
	74.21	73.51	73.26	180.84	178.04	178.45
	76.92	73.65	73.74	180.89	180.54	180.39
	77.50	75.35	74.48	182.45	180.68	180.61
	77.68	76.92	76.65	182.97	182.60	182.58
	78.50	77.04	77.06	183.80	182.86	182.91

80.23	77.58	77.48	184.28	183.62	183.37
81.23	78.85	78.77	186.20	184.22	183.69
83.17	80.46	80.89	186.82	186.66	186.18
83.58	81.39	81.81	187.30	186.95	186.65
88.62	83.56	83.66	189.57	187.35	187.71
89.01	84.14	84.14	190.78	188.91	188.67
89.49	88.59	87.30	192.46	190.66	190.73
90.31	89.16	88.65	193.34	192.11	191.82
90.46	89.69	89.23	193.98	192.65	193.15
91.03	89.83	89.60	194.49	193.87	193.76
91.51	90.59	90.09	196.12	194.42	194.06
91.91	91.13	90.94	197.39	196.70	196.22
92.01	91.32	91.36	197.94	196.96	196.47
95.19	91.90	91.45	199.20	197.91	197.85
95.30	92.05	92.09	199.53	198.87	199.26
97.33	94.72	92.18	202.46	199.75	199.30
98.55	94.93	94.70	202.82	202.10	201.01
99.54	97.91	94.96	203.41	202.86	202.62
99.77	98.58	97.77	207.59	203.56	203.34
100.21	99.29	98.39	207.83	207.14	206.78
101.29	100.03	99.31	208.08	207.89	207.91
102.15	100.12	100.03	209.76	208.13	208.31
103.01	101.19	100.42	209.94	209.96	208.95
103.44	101.72	101.53	210.57	210.07	210.36
105.04	103.22	101.88	213.63	210.71	210.43
105.98	104.21	103.17	214.18	214.00	214.40
106.91	104.52	103.71	215.13	214.92	214.82
107.94	105.70	104.60	218.44	215.46	215.57
108.38	106.95	105.83	218.79	218.52	217.85
108.87	107.86	106.62	218.93	218.61	218.64
110.45	108.00	107.60	219.17	219.23	219.16
110.70	108.71	108.47	221.70	219.38	219.36
110.85	110.49	108.71	223.00	222.02	222.19
112.76	111.01	110.58	229.36	223.05	222.63
113.19	111.21	111.12	229.86	229.77	229.40
113.54	113.10	112.06	233.49	229.90	229.83
114.06	113.43	112.98	242.28	234.07	234.46
114.70	114.02	113.37	243.35	242.06	240.55
114.98	114.65	114.20	246.29	243.18	241.97
115.76	115.13	114.62	248.02	246.06	244.29
117.33	116.19	114.99	249.45	248.16	245.56
117.46	116.91	116.03	249.77	249.68	246.33
118.24	117.23	116.95	250.70	249.73	248.26
118.49	118.21	117.75	251.71	250.59	249.15

118.72	118.41	118.21		253.63	251.05	249.41
119.05	118.79	118.21		253.70	252.96	250.90
119.42	119.12	118.71		254.29	253.04	250.95
119.86	119.85	118.84		254.68	254.06	252.24
120.12	120.08	119.53		256.31	254.65	253.07
120.98	120.44	119.78		256.81	255.45	253.26
121.53	120.97	120.01		257.85	255.99	253.96
121.81	121.46	120.74		259.05	257.33	254.39
122.66	121.88	121.40		260.68	258.61	254.92
124.26	122.34	121.74		261.69	260.48	259.38
125.70	124.27	121.94		263.88	260.81	261.38
126.09	125.84	124.17		267.04	263.27	261.67
126.42	125.88	125.44		559.87	267.48	268.98
127.09	126.46	125.98		595.36	408.40	347.67
127.42	126.74	126.02		930.39	489.55	541.29
128.63	127.25	126.54		3598.66	3570.36	3521.21
128.90	128.51	127.31	V/Cu(320)	11.88	-1982.05	12.26
129.67	128.83	128.49		15.54	15.90	15.77
129.86	129.33	128.79		16.56	16.38	17.08
130.60	129.59	129.24		17.03	24.18	23.69
131.92	130.20	129.47		24.44	25.29	24.63
133.21	132.05	130.19		25.38	26.12	25.24
135.29	132.83	131.96		26.46	33.62	31.05
137.34	135.35	132.72		34.01	35.24	32.75
137.87	136.46	135.69		35.52	37.19	34.19
138.31	137.21	137.09		37.34	37.87	35.05
138.61	137.90	137.55		38.27	47.94	36.84
139.17	138.66	138.24		49.00	49.81	37.78
140.06	138.87	138.54		49.77	50.85	49.06
140.91	140.37	138.68		53.45	53.37	49.28
141.84	140.59	140.30		54.17	54.17	51.53
143.69	141.52	140.59		54.33	54.75	53.19
145.86	142.28	141.36		55.15	55.47	54.03
146.24	144.52	143.92		55.68	57.48	54.84
147.13	145.96	145.55		57.47	57.53	55.21
147.57	146.38	146.04		57.99	58.06	57.54
148.08	147.20	147.03		58.76	59.31	57.70
148.47	147.65	147.55		59.36	62.07	58.53
148.85	148.05	147.89		62.85	62.91	60.26
149.26	148.48	148.29		63.37	63.53	62.23
149.81	148.62	148.53		63.62	63.68	62.76
149.93	149.26	148.98		63.96	64.26	63.43
150.76	149.97	149.59		64.58	64.55	63.91
151.77	150.10	149.86		65.16	64.98	64.09

152.88	151.19	150.75	65.53	65.62	64.62
153.24	152.17	151.73	66.44	66.83	65.51
153.72	153.11	152.75	67.40	67.45	65.82
154.86	153.45	153.26	67.66	68.51	67.02
155.11	153.65	153.45	69.68	69.69	67.67
155.57	155.04	154.67	69.99	70.13	68.64
157.13	155.43	155.44	70.24	70.72	69.65
159.57	155.89	155.86	71.29	71.31	70.22
160.26	157.04	156.97	71.48	71.65	70.89
161.85	159.82	159.51	72.05	74.94	71.20
162.49	160.61	160.22	75.28	75.37	71.78
162.78	162.28	161.81	76.35	76.62	75.16
162.98	162.51	162.03	77.95	78.01	75.71
163.36	163.13	162.43	79.60	79.64	78.40
164.07	163.20	162.68	80.84	81.10	79.36
164.48	163.53	163.20	81.74	82.78	80.73
164.63	164.33	163.45	85.86	85.14	81.18
165.48	164.66	164.25	88.00	87.98	87.58
168.44	164.88	164.34	89.09	88.78	88.11
169.52	165.70	164.89	90.13	90.16	89.69
170.48	168.92	168.28	90.46	90.74	90.05
171.89	169.61	169.14	91.02	91.25	90.66
173.15	170.78	170.32	91.85	91.94	90.86
173.33	171.97	171.85	92.27	92.26	91.36
174.08	173.24	173.05	92.91	93.10	91.97
175.73	173.63	173.35	93.59	93.77	92.58
176.35	174.06	173.83	94.52	94.63	93.49
176.86	176.21	175.51	94.96	95.19	94.30
177.24	176.74	176.43	95.87	95.81	94.92
178.44	177.45	176.76	96.83	96.54	95.66
178.59	177.53	177.04	97.14	96.85	95.80
179.29	178.50	178.17	97.41	98.03	96.89
179.76	178.75	178.29	98.31	98.29	97.12
180.11	179.51	178.93	99.05	99.02	97.58
180.90	180.06	179.46	102.25	102.24	100.63
181.12	180.80	180.46	102.92	102.92	101.94
181.81	181.12	181.03	103.02	103.08	102.21
184.36	181.79	181.31	103.74	103.67	103.11
185.36	182.86	182.33	104.30	104.23	103.64
186.47	184.89	184.35	104.61	104.41	104.11
187.05	185.87	185.41	105.78	105.45	104.34
188.31	186.67	186.20	106.40	106.40	105.38
188.75	187.46	186.92	107.17	106.98	106.37
189.01	188.66	187.96	107.32	107.27	106.69

189.81	189.21	188.31	110.52	110.15	107.20
190.23	189.33	189.00	111.16	110.59	108.88
192.84	189.98	189.22	111.64	111.70	110.23
193.66	190.24	189.63	112.43	112.45	111.26
195.49	192.36	191.22	113.11	113.04	112.00
196.25	193.19	192.64	113.92	113.89	112.42
196.77	194.01	193.57	114.19	114.03	112.83
198.02	195.43	194.72	114.36	114.35	113.67
200.33	196.73	196.21	114.99	114.82	113.83
200.63	198.19	197.97	115.06	114.93	114.36
201.81	198.91	198.13	115.16	114.98	114.51
203.34	200.33	199.95	115.69	115.53	114.58
203.98	201.67	201.23	115.95	115.62	115.07
204.38	203.19	202.68	116.36	116.31	115.26
205.88	203.80	203.12	116.42	116.41	115.51
206.75	204.34	203.62	116.84	116.57	115.95
206.83	205.33	204.47	116.90	117.05	116.16
208.43	206.74	206.20	117.35	117.11	116.25
208.79	207.04	206.47	117.49	117.36	116.68
209.16	207.92	206.78	120.05	119.91	117.12
209.78	208.57	207.86	121.17	120.85	119.30
212.05	209.22	208.83	121.56	121.40	120.68
212.86	209.91	209.13	122.02	121.72	120.98
213.30	210.85	209.96	124.07	123.40	121.25
213.59	212.33	211.74	124.82	124.62	122.18
214.23	212.96	212.47	125.98	125.97	123.51
215.63	213.48	212.92	127.00	126.79	125.52
215.93	213.85	213.55	127.11	127.05	126.31
216.43	215.32	214.79	127.35	127.47	126.48
216.87	216.07	215.68	128.14	127.76	126.84
217.60	216.56	215.93	128.43	128.34	127.52
217.66	216.96	216.46	129.03	128.66	127.96
218.55	217.68	217.05	129.19	129.08	128.47
219.11	217.87	217.33	130.08	130.00	128.80
219.64	218.31	217.75	131.48	131.49	129.46
220.20	219.07	218.42	132.40	132.46	130.25
221.03	219.28	218.84	133.14	133.04	132.20
221.47	220.07	219.54	136.91	136.41	132.64
221.83	220.87	220.46	137.61	137.53	136.14
222.31	221.24	220.65	137.84	137.77	137.03
223.28	221.56	221.21	138.39	138.22	137.32
223.66	222.38	222.04	139.18	138.97	137.45
224.86	223.28	222.92	139.56	139.93	138.68
226.08	223.46	223.05	141.32	141.17	139.08

	226.67	224.75	224.51	141.75	141.79	140.88
	226.81	226.23	225.69	142.49	142.55	141.15
	227.25	226.55	226.06	144.95	144.71	142.33
	228.11	226.69	226.10	145.16	145.15	144.01
	228.23	227.36	226.77	146.42	146.11	144.63
	229.23	227.70	226.92	147.37	146.87	145.74
	229.50	228.31	227.76	147.93	147.40	146.66
	230.50	229.24	228.11	148.30	148.08	147.08
	230.76	229.35	228.83	148.50	148.47	147.76
	231.79	230.54	229.71	148.96	148.75	147.78
	232.03	230.65	230.23	149.56	149.71	148.06
	232.57	231.74	231.01	150.21	150.22	149.32
	232.98	231.97	231.35	151.12	151.15	149.58
	233.47	232.24	231.78	152.26	152.12	150.21
	235.00	232.77	232.28	153.35	153.36	151.82
	235.52	233.16	232.43	154.33	154.21	152.79
	236.39	234.56	233.62	154.83	155.09	153.77
	237.36	235.02	234.49	155.62	155.52	154.08
	237.94	236.52	235.74	158.03	156.71	155.24
	238.22	236.57	235.98	158.56	158.26	155.48
	238.91	237.97	237.28	160.21	160.09	157.50
	240.10	238.10	237.64	160.86	160.61	159.57
	240.92	239.27	238.48	161.22	161.21	160.03
	365.44	240.03	239.01	161.75	161.62	160.28
	390.96	240.40	239.87	161.91	161.98	161.12
	643.05	339.83	334.44	162.17	162.20	161.27
	692.43	384.59	447.33	162.75	162.63	161.46
	3528.02	3548.00	3516.22	163.36	162.95	162.09
Nb/Cu(320)	13.90	-1776.56	13.30	164.00	163.87	162.67
	16.31	15.34	17.06	164.85	164.75	163.39
	17.93	16.56	17.26	167.99	167.70	163.55
	23.75	23.78	22.91	168.35	168.08	166.78
	25.76	25.84	25.23	169.10	168.94	167.70
	26.38	26.16	25.48	170.44	170.45	168.55
	30.65	30.84	27.22	171.11	171.09	169.92
	35.31	35.16	30.57	171.43	171.35	170.38
	36.51	36.55	33.84	171.86	171.54	170.61
	37.88	37.61	34.82	173.56	172.15	171.15
	41.99	44.98	36.30	174.37	174.17	171.37
	46.41	48.24	37.32	174.64	174.55	173.57
	48.09	49.88	48.36	174.78	174.85	173.90
	49.98	53.95	48.95	175.88	175.54	173.98
	53.87	54.12	49.89	176.82	176.52	175.09
	54.22	54.76	53.65	177.09	176.97	175.74

54.69	55.04	53.95	177.32	177.26	176.67
55.28	57.08	54.67	178.19	178.37	176.88
56.85	57.44	55.02	180.93	180.80	177.86
57.39	58.20	57.02	181.09	181.04	179.73
58.47	58.88	57.32	182.68	182.43	180.53
59.19	61.70	58.27	183.43	183.38	181.80
61.58	62.77	59.12	184.29	184.08	182.60
62.69	63.28	61.88	184.89	184.85	183.65
63.29	63.60	62.24	185.20	185.19	184.43
63.52	64.05	63.18	186.16	185.91	184.53
64.15	64.31	63.87	187.50	187.29	185.61
64.91	64.87	63.87	187.68	187.55	186.83
65.08	65.59	64.38	189.15	188.92	186.94
65.71	66.83	65.16	191.25	191.18	188.60
67.02	67.80	65.55	192.20	192.19	190.59
67.89	68.32	66.92	192.55	192.53	191.09
68.41	69.57	67.85	193.54	193.17	192.10
69.67	70.04	68.51	194.87	194.78	192.81
69.93	70.64	69.43	196.78	196.88	194.11
70.76	71.15	70.05	198.23	197.89	196.21
71.40	71.53	70.73	198.53	198.57	197.11
71.65	74.51	71.03	199.77	200.02	197.87
74.78	74.79	71.46	201.19	200.87	199.34
75.60	75.59	74.80	202.04	202.01	200.52
78.00	78.13	75.40	202.66	202.44	201.24
79.33	79.80	78.28	203.34	202.81	201.60
80.13	81.24	79.28	203.76	203.63	202.06
80.98	81.48	80.45	204.20	203.93	203.11
85.85	86.26	81.21	204.74	204.47	203.40
87.06	87.64	86.47	205.87	205.50	203.93
88.40	88.45	87.84	206.94	206.69	204.97
89.82	89.89	89.60	207.45	207.25	206.02
90.58	90.90	89.95	208.06	208.06	206.74
90.77	91.17	90.75	209.15	209.06	207.16
91.07	91.71	91.11	211.26	211.06	208.37
91.53	92.06	91.42	212.67	212.47	210.69
92.13	92.24	91.68	212.75	212.75	211.75
93.86	93.92	92.37	213.10	212.96	212.02
94.24	94.50	93.91	214.63	214.29	212.47
94.93	94.80	94.26	214.95	214.65	213.78
95.44	95.56	94.85	215.32	215.30	214.21
95.97	96.22	95.14	215.48	215.42	214.50
96.82	96.50	95.69	215.76	215.59	214.71
97.09	97.81	96.59	216.43	216.22	215.15

98.04	98.51	97.31		217.52	217.25	215.54
98.46	98.98	97.98		218.50	218.43	216.89
101.60	101.87	101.45		218.70	218.58	217.65
102.39	102.36	101.71		219.74	219.87	217.97
102.61	102.82	102.46		220.75	220.78	219.22
103.79	103.67	103.05		221.09	221.01	220.20
103.95	104.14	103.62		221.49	221.39	220.40
104.28	104.20	103.89		221.93	221.88	220.81
105.13	105.59	104.32		222.55	222.44	221.43
106.22	106.13	105.51		222.73	222.68	221.89
106.31	106.64	106.18		224.10	223.91	222.14
106.58	107.10	106.31		224.37	224.49	223.40
107.51	108.92	107.33		224.96	224.95	223.94
111.63	111.83	111.30		226.02	225.98	224.35
112.26	112.27	111.73		226.61	226.43	225.24
112.71	112.89	111.98		226.77	226.78	226.03
113.04	113.15	112.83		228.50	228.37	226.43
113.53	114.08	112.92		228.95	228.84	227.86
114.22	114.45	113.63		229.11	228.95	228.14
114.64	114.63	114.06		229.70	229.71	228.62
114.82	114.86	114.31		230.11	230.05	229.04
115.09	115.05	114.66		230.62	230.34	229.54
115.21	115.23	114.72		230.81	230.77	229.95
115.27	115.36	114.92		231.16	231.03	230.21
115.37	115.74	115.05		231.47	231.41	230.53
115.96	115.97	115.39		233.11	233.15	230.82
116.37	116.21	115.62		236.17	236.08	232.58
116.63	116.47	116.23		236.52	237.16	235.49
116.92	116.83	116.54		238.11	237.92	236.42
117.29	117.24	116.69		238.86	238.65	237.42
117.95	117.59	116.99		238.98	238.88	238.05
120.01	120.03	119.56		239.25	239.16	238.31
121.06	121.11	120.64		239.63	239.59	238.65
121.14	121.52	120.85		240.54	240.45	238.83
122.31	122.62	121.79		242.04	242.18	239.71
122.74	122.83	122.09		399.92	315.35	241.53
125.74	125.71	124.83		479.17	420.22	384.49
125.81	125.78	125.47		965.72	469.34	479.27
126.23	126.56	126.25		3559.09	3588.77	3534.32
127.14	127.03	126.63	Ta/Cu(320)	6.46	-1497.68	15.91
127.53	127.40	127.13		18.48	8.46	18.03
128.03	128.00	127.67		19.83	19.32	18.34
128.47	128.37	128.03		23.97	24.02	24.69
128.81	128.51	128.20		25.27	25.27	26.94

130.05	129.75	129.53	27.32	26.75	27.22
130.82	130.92	130.29	27.85	28.06	27.65
131.66	131.37	131.23	30.72	30.77	30.75
132.46	132.59	132.29	33.01	33.16	33.23
133.56	133.08	132.88	34.34	34.08	34.29
136.83	137.02	136.59	38.59	36.96	38.73
137.56	137.50	137.16	44.99	45.27	45.42
138.10	138.07	137.59	45.66	45.92	48.92
138.61	138.18	137.72	48.82	49.47	52.02
138.96	138.98	138.60	50.47	52.33	52.06
140.08	139.98	139.68	52.42	53.56	53.82
141.71	141.72	141.34	53.64	54.35	55.42
142.02	141.88	141.50	55.66	56.59	57.81
142.90	142.84	141.67	56.72	57.80	59.01
144.61	144.63	142.76	58.83	59.10	59.58
145.82	145.64	144.09	59.56	59.65	59.83
146.96	146.88	145.27	59.76	59.87	59.85
147.45	147.43	146.60	60.34	60.99	60.95
148.14	148.05	147.05	61.15	61.24	61.23
148.57	148.57	147.80	61.41	61.50	61.52
148.80	148.84	147.97	63.35	63.55	63.27
149.56	149.29	148.23	65.43	65.65	65.21
150.36	150.35	148.79	66.31	67.02	66.93
150.99	150.73	150.05	67.04	67.39	67.51
151.28	151.33	150.42	67.57	68.46	67.68
153.11	153.02	150.67	68.52	68.88	68.44
154.08	154.04	152.44	69.67	69.57	69.42
154.43	154.41	153.46	69.80	69.85	69.83
154.67	154.80	153.70	70.44	70.89	70.25
156.54	156.50	153.85	70.76	71.05	71.05
158.21	158.02	156.52	71.10	71.65	71.43
158.69	158.34	156.62	74.28	74.44	73.73
160.16	160.24	157.48	74.36	74.60	74.11
160.94	161.04	159.80	76.39	76.86	76.95
161.36	161.46	160.71	77.73	78.20	77.79
161.74	161.83	160.88	78.47	78.47	78.70
161.98	161.91	161.35	79.94	80.16	79.54
162.06	162.21	161.40	81.49	81.45	80.24
163.10	162.76	161.44	81.52	81.85	81.59
163.78	163.85	162.28	84.93	85.63	83.09
164.44	164.43	163.43	85.54	86.54	87.00
166.36	165.42	163.64	89.25	89.36	88.58
168.43	168.25	165.60	89.45	89.64	89.27
168.70	168.58	167.88	90.11	90.20	90.02

169.32	169.33	168.11	90.56	90.45	90.07
170.82	170.76	168.79	90.89	90.97	90.57
171.32	171.36	170.22	91.36	91.30	90.96
171.75	171.58	170.77	92.55	92.72	91.77
172.06	171.84	171.08	93.67	93.78	92.46
174.16	174.14	171.70	94.07	94.08	93.84
174.36	174.32	173.24	95.33	95.18	94.07
174.74	174.40	173.76	95.71	95.76	95.07
175.25	175.26	173.82	97.26	96.93	95.55
176.11	176.03	174.53	97.46	97.24	96.79
176.92	176.92	175.38	99.57	98.00	97.23
177.50	177.26	176.56	100.41	100.64	99.51
178.75	178.71	176.91	101.75	101.10	100.50
179.42	179.15	178.34	101.88	101.85	101.08
181.06	180.98	178.58	102.86	102.41	101.87
181.82	181.77	180.51	103.81	103.35	102.76
183.44	183.41	181.19	104.67	104.33	103.48
184.41	184.46	182.87	105.98	106.27	105.51
184.79	184.81	183.77	106.71	106.56	106.25
185.33	185.28	184.31	107.44	106.95	106.45
186.28	185.78	184.60	107.61	107.50	107.17
187.50	187.32	184.97	109.23	108.20	107.64
187.63	187.54	186.72	109.46	109.19	108.44
188.50	188.40	187.09	109.52	109.42	109.13
190.60	190.05	187.96	111.21	110.33	109.31
192.19	192.13	189.44	111.48	111.15	109.70
192.50	192.43	191.76	112.45	111.38	110.41
193.32	193.75	191.99	112.94	112.81	110.77
194.42	194.14	192.64	114.84	112.99	112.30
194.95	194.80	193.59	115.54	115.18	112.79
197.92	197.74	194.49	116.36	115.72	114.99
198.30	198.25	196.73	117.04	116.58	115.60
199.37	199.46	197.66	117.27	117.14	116.33
200.55	200.78	198.66	117.53	117.27	116.81
202.05	201.93	200.31	118.10	117.72	116.93
202.58	202.52	201.17	118.18	118.12	117.23
203.04	202.65	201.33	118.89	118.26	117.65
203.32	203.13	201.81	119.04	118.77	117.95
203.99	203.83	202.06	119.33	119.06	118.22
204.80	204.45	203.18	120.05	119.33	118.71
205.37	205.07	203.92	120.67	120.12	118.94
206.85	206.66	204.10	121.89	120.51	119.56
207.30	207.06	205.81	122.04	121.89	120.35
208.11	207.82	206.18	123.14	122.02	121.54

208.90	208.60	207.16	123.75	123.16	121.85
209.61	209.25	207.90	124.09	123.57	122.67
212.04	212.00	208.33	124.85	124.15	122.85
212.54	212.34	211.34	124.98	124.77	123.86
212.72	212.52	211.71	125.20	124.87	124.00
213.47	213.22	211.91	126.03	124.99	124.17
214.23	213.89	212.61	126.60	125.98	124.68
214.94	214.80	213.11	127.23	126.59	125.74
215.34	214.95	213.98	127.78	127.25	126.44
215.63	215.44	214.38	128.44	127.84	126.98
216.06	215.76	214.95	128.91	128.49	127.51
216.39	216.17	215.24	131.13	128.91	128.10
217.67	217.52	215.57	131.55	130.67	128.63
218.30	217.96	216.83	133.49	131.37	130.73
218.84	218.62	217.42	134.34	133.61	130.85
220.15	220.39	218.06	135.52	134.50	133.38
220.74	220.80	219.85	135.86	135.43	134.63
221.54	221.49	220.37	138.52	135.85	135.00
221.74	221.69	221.00	139.31	138.48	135.54
221.85	221.91	221.21	140.99	139.51	138.34
222.66	222.62	221.42	141.13	140.75	139.06
222.97	222.89	222.16	142.24	141.27	140.39
224.42	224.37	222.46	142.70	142.11	140.73
224.79	224.67	223.80	143.65	142.56	141.77
225.66	225.49	224.13	143.93	143.66	142.22
226.23	226.14	224.90	144.45	143.84	143.38
226.43	226.60	225.42	144.64	144.46	143.45
227.26	227.28	226.20	144.96	144.72	144.17
228.83	228.47	226.94	145.40	144.89	144.40
229.25	229.30	228.14	145.73	145.42	144.72
229.52	229.41	228.70	146.66	145.80	145.41
230.08	229.91	228.89	146.89	146.57	145.61
230.44	230.06	229.49	148.66	146.94	146.14
230.60	230.58	229.68	148.97	148.68	146.89
231.28	230.95	230.09	149.22	148.99	148.67
232.46	232.11	230.67	149.93	149.50	148.98
232.52	232.32	231.33	151.36	150.05	149.43
233.24	233.44	231.48	151.49	151.40	149.77
237.74	237.67	233.00	152.17	152.03	151.27
238.34	238.27	237.09	153.12	152.31	151.65
238.70	238.64	237.67	154.80	153.75	152.16
238.98	238.87	238.15	157.01	154.89	153.37
239.37	239.19	238.25	157.92	157.46	154.59
239.44	239.43	238.67	158.56	158.16	157.01

	240.38	240.08	238.92	158.88	158.71	157.66
	241.07	241.09	239.51	159.74	159.51	158.28
	243.09	243.00	240.16	160.44	159.90	159.46
	418.97	271.05	242.49	160.75	160.58	159.72
	502.89	404.08	349.50	161.68	160.85	160.44
	887.56	421.21	469.44	162.11	161.69	160.58
	3563.94	3592.71	3523.10	163.13	162.30	161.42
W/Cu(320)	6.60	-1358.43	6.93	164.49	163.19	162.14
	10.23	7.97	9.70	165.64	164.31	163.02
	10.40	12.52	11.70	168.59	168.48	164.50
	20.38	28.05	27.23	169.19	169.01	168.01
	27.65	28.48	27.62	169.76	169.71	168.91
	28.26	30.92	28.27	171.49	171.30	169.78
	31.53	30.88	31.52	171.97	171.86	171.08
	33.32	31.79	37.02	172.49	172.23	171.62
	37.01	36.83	38.72	173.60	173.27	171.94
	40.45	40.47	39.92	173.78	173.63	173.02
	40.88	40.88	40.54	173.98	173.84	173.24
	44.17	45.71	44.97	174.22	173.99	173.52
	49.44	49.30	47.34	174.81	174.25	173.75
	52.27	52.37	52.17	175.82	175.57	173.99
	56.88	56.86	53.79	176.43	175.85	175.29
	57.92	57.66	57.09	177.58	177.37	175.68
	58.20	58.29	57.92	178.70	178.66	177.28
	59.81	59.98	58.42	179.07	178.92	178.47
	61.28	61.35	59.72	180.94	180.75	178.65
	61.71	61.64	60.69	181.28	181.25	180.49
	62.15	63.29	61.39	182.29	181.90	180.91
	63.41	63.63	63.25	183.02	183.06	181.65
	63.49	63.85	63.38	183.30	183.28	182.59
	63.77	64.09	63.49	184.43	184.26	182.82
	64.18	64.24	63.90	185.95	185.01	183.72
	64.52	66.46	64.23	187.90	187.74	184.52
	66.38	66.81	64.52	188.28	188.30	187.43
	67.23	67.32	66.54	188.59	188.43	187.97
	67.39	67.79	66.82	189.16	188.83	188.14
	67.67	68.13	67.09	189.18	189.21	188.68
	68.09	69.33	67.68	190.67	190.16	189.14
	69.30	69.79	67.93	190.94	191.17	190.15
	70.45	70.91	69.10	192.90	192.75	190.35
	71.36	71.98	70.00	193.27	193.20	192.78
	72.03	72.19	71.19	195.61	195.72	193.22
	72.20	72.99	72.18	196.76	196.96	195.33
	73.05	74.98	72.80	197.74	197.91	196.05

75.04	76.33	73.30	199.13	199.00	197.85
76.05	77.21	75.17	199.32	199.11	198.59
77.20	77.44	75.92	199.81	199.80	198.79
77.57	79.77	76.93	200.20	200.03	199.36
80.61	80.97	77.30	201.36	201.19	199.44
81.48	82.37	80.47	201.87	201.65	200.87
83.13	83.52	81.41	203.58	203.43	201.45
83.62	85.09	82.82	203.89	203.88	203.28
85.41	88.54	83.32	206.30	206.43	203.53
88.19	89.11	87.27	206.55	206.53	205.96
89.53	90.11	88.02	207.09	206.95	206.24
90.11	90.84	89.45	208.00	207.96	206.62
90.68	91.46	90.32	208.83	208.83	207.38
91.43	92.09	90.71	210.93	210.93	208.70
92.20	92.56	91.39	211.35	211.32	210.49
93.30	93.24	92.29	212.26	212.10	210.95
93.83	94.52	92.93	212.53	212.30	211.64
94.27	94.68	93.84	213.32	213.32	211.86
94.66	95.83	94.42	214.38	214.25	212.97
97.83	98.34	94.76	215.00	215.09	213.78
98.54	99.01	97.57	215.55	215.48	214.80
99.20	99.49	98.32	215.77	215.66	215.10
99.46	99.72	98.67	216.09	216.15	215.41
100.12	100.27	99.56	216.71	216.54	215.62
101.04	100.99	100.16	216.98	216.81	216.09
101.77	101.90	100.40	217.06	216.84	216.20
101.96	102.19	101.44	219.66	219.50	216.49
103.31	103.36	102.10	220.02	219.96	219.09
103.84	104.39	102.92	220.38	220.56	219.64
104.51	104.44	103.63	220.52	220.60	220.15
105.68	105.52	104.24	221.23	221.20	220.36
106.59	106.59	105.38	222.01	221.70	220.87
107.00	107.01	106.46	222.34	222.48	221.43
108.97	109.03	106.70	224.26	224.23	222.20
109.57	109.54	108.90	224.89	224.61	223.96
109.87	109.69	109.46	226.31	226.07	224.32
111.79	112.24	109.64	226.77	226.69	225.49
113.17	113.05	111.88	227.15	227.23	226.28
114.02	114.31	112.95	227.35	227.42	227.05
114.52	114.65	114.26	228.28	228.13	227.21
114.80	114.89	114.51	229.81	229.97	228.02
116.61	116.64	114.79	229.94	230.02	229.47
116.91	116.91	116.37	230.44	230.38	229.72
117.83	118.18	116.44	231.09	231.05	229.97

118.13	118.29	117.49		231.85	231.72	230.90
118.40	118.61	118.11		232.52	232.45	231.59
118.90	118.97	118.25		232.68	232.50	232.20
119.17	118.99	118.56		233.28	233.16	232.32
119.36	119.55	118.79		233.65	233.53	233.06
120.03	120.04	119.00		236.25	236.18	233.51
120.53	120.70	119.83		236.45	236.35	235.58
120.89	120.95	119.93		237.05	236.94	235.79
121.24	121.28	120.70		237.59	237.54	236.47
121.43	121.44	121.02		237.88	238.26	237.07
121.74	121.55	121.22		238.52	238.55	237.86
123.65	123.59	121.59		238.89	238.82	238.47
124.20	124.22	122.99		239.52	240.08	238.63
124.90	124.70	123.62		240.60	241.16	240.03
125.28	125.12	124.35		463.96	256.21	241.38
126.54	126.58	124.78		512.67	413.76	348.97
127.15	127.43	126.55		903.69	473.10	483.27
128.04	128.24	127.18		3602.68	3591.97	3510.19
128.63	128.61	127.81	V/Cu(553)	11.51	-2266.13	11.35
128.88	129.05	128.44		21.96	11.43	21.84
130.05	130.08	128.77		31.83	22.16	26.93
130.55	130.22	129.76		38.05	27.41	31.89
131.35	130.88	130.27		42.67	31.84	38.47
132.56	132.51	131.02		44.80	38.34	43.21
133.44	133.47	132.55		52.43	42.82	45.30
133.93	133.53	133.12		53.75	45.02	51.49
136.07	135.97	133.25		54.05	52.54	52.94
136.48	136.62	135.81		58.89	53.81	53.83
139.32	139.03	136.32		59.76	53.86	57.11
139.62	139.57	138.99		60.47	59.04	59.22
140.36	140.37	139.47		63.14	59.73	59.91
141.11	141.07	140.33		65.16	60.27	62.83
141.34	141.19	140.95		67.23	63.09	64.85
142.20	141.93	141.27		67.49	65.09	65.24
144.15	143.99	142.14		67.77	66.49	67.38
145.42	145.74	143.42		69.85	67.22	67.83
146.86	147.06	145.45		70.01	67.41	68.90
147.18	147.15	146.71		70.10	67.98	69.80
147.83	147.43	146.86		70.41	69.75	70.12
148.52	148.69	147.42		71.06	70.08	70.26
149.02	149.11	148.51		73.04	70.33	70.77
149.36	149.35	149.10		76.48	70.39	71.21
149.57	149.66	149.15		76.86	71.14	73.24
150.33	150.17	149.37		77.47	73.18	76.69

151.27	151.06	150.16	77.49	76.49	76.72
151.78	151.88	151.01	78.01	76.76	76.98
152.55	152.14	151.75	79.48	77.36	77.52
153.85	153.82	152.13	82.28	77.68	77.63
155.18	154.88	153.83	82.45	77.83	79.57
155.22	155.43	154.76	84.44	79.55	82.15
156.05	156.25	155.18	84.66	82.24	82.61
157.10	157.23	155.79	85.44	82.53	84.38
157.54	157.69	157.06	85.64	84.39	84.56
158.35	158.38	157.35	86.34	84.60	85.83
161.21	161.50	158.50	86.49	85.54	86.37
161.81	161.67	161.20	87.43	86.37	86.45
162.34	162.37	161.36	90.24	86.51	87.48
162.60	162.71	162.00	92.54	87.45	90.66
162.89	162.86	162.23	93.14	90.60	92.73
163.31	163.17	162.56	94.19	92.77	93.00
163.44	163.46	162.84	94.64	93.02	94.46
164.15	164.39	162.95	94.89	94.31	94.58
165.04	164.90	163.79	95.37	94.64	94.83
166.72	165.87	164.92	95.42	95.08	95.08
166.86	166.82	166.05	96.69	95.49	95.94
169.06	169.10	166.75	97.06	95.52	96.75
169.67	169.68	168.84	97.17	96.55	96.84
171.76	171.84	169.41	98.35	96.82	97.00
173.28	173.40	171.35	98.37	97.17	98.82
173.80	173.73	173.01	99.16	98.46	99.11
174.51	174.51	173.55	99.78	98.53	99.41
175.28	174.92	174.34	99.86	99.27	100.08
176.51	176.41	174.87	100.72	99.86	100.23
176.63	176.69	176.22	100.78	100.01	100.42
177.75	177.95	176.50	100.94	100.68	100.77
178.20	178.15	177.55	101.21	100.80	100.84
178.51	178.37	177.86	101.45	100.88	101.17
178.92	178.90	178.06	101.67	101.06	101.32
179.27	179.52	178.78	101.73	101.60	101.80
181.41	181.71	179.07	102.26	101.71	101.84
181.99	181.98	181.52	102.43	101.85	102.28
182.14	182.31	181.79	102.72	102.20	102.64
182.67	182.78	181.83	102.94	102.77	102.81
182.98	183.34	182.38	103.66	102.86	103.52
185.90	185.89	183.12	106.16	103.33	104.24
186.87	186.85	185.61	106.33	103.53	105.97
187.66	187.46	186.59	106.46	106.11	106.62
188.40	188.21	187.03	107.11	106.35	106.86

189.71	189.58	187.70	108.03	106.58	107.36
189.77	189.73	189.23	108.07	107.19	107.84
190.70	190.71	189.43	108.65	107.22	108.13
191.10	191.09	190.50	109.18	108.49	108.45
192.08	192.28	190.73	110.68	109.58	110.15
193.26	193.30	191.75	110.87	110.40	110.69
194.48	194.31	193.22	111.44	110.86	111.19
196.58	196.50	193.96	111.80	111.52	111.71
197.04	196.91	196.36	112.99	111.66	111.92
197.56	197.66	196.99	113.31	112.74	112.57
199.74	199.59	197.26	113.45	113.29	113.38
200.08	199.98	199.27	113.90	113.41	113.67
200.84	201.14	199.65	114.14	113.55	113.78
203.28	203.31	200.83	114.23	114.28	114.48
204.42	204.39	202.99	115.05	114.65	114.63
204.52	204.41	203.79	115.37	114.73	115.14
205.52	205.23	203.89	115.49	115.45	115.41
206.02	206.05	204.95	116.17	115.54	115.77
206.69	206.67	205.76	116.53	115.98	115.96
207.02	207.09	206.19	117.06	116.19	116.39
208.38	208.10	206.58	117.76	116.79	116.93
208.79	208.53	207.77	118.03	117.51	117.66
209.19	208.97	208.09	119.18	117.98	117.98
209.58	209.56	208.80	119.44	119.06	118.80
211.05	210.86	209.19	119.53	119.43	119.18
213.44	213.45	210.73	120.19	119.51	119.58
213.89	213.65	213.15	121.30	119.88	120.74
214.11	213.92	213.41	121.46	121.24	121.16
214.65	214.66	213.77	121.76	121.46	121.52
216.01	215.86	214.39	122.03	121.72	121.83
216.43	216.51	215.38	122.21	121.89	121.96
216.97	216.85	216.21	122.73	122.18	122.20
217.40	217.42	216.67	122.86	122.59	122.62
217.78	217.54	217.12	123.20	122.78	123.01
218.33	218.08	217.24	123.42	123.15	123.11
218.60	218.50	217.72	123.56	123.33	123.29
219.03	218.96	218.36	123.88	123.51	123.58
219.65	219.71	218.54	123.94	123.77	123.76
220.85	221.01	219.54	124.33	123.98	123.93
221.84	221.92	220.85	124.72	124.07	124.03
222.28	222.16	221.72	125.50	124.51	124.56
222.40	222.66	221.91	125.66	125.29	125.40
222.98	223.09	222.48	125.95	125.57	125.64
224.22	224.24	222.89	127.16	126.16	126.32

	224.51	224.43	223.87	127.98	127.58	127.87
	226.40	226.24	224.09	128.14	127.82	127.92
	226.56	226.92	226.05	128.75	128.10	128.27
	227.11	227.20	226.64	128.95	128.31	128.38
	227.28	227.61	226.78	129.70	128.85	128.98
	227.85	227.67	227.22	129.97	129.71	129.56
	229.33	229.40	227.66	130.54	130.01	129.72
	229.58	229.69	228.86	130.89	130.31	130.61
	229.84	230.00	229.46	131.27	130.66	130.88
	230.30	230.35	229.84	131.91	131.01	130.99
	230.78	230.86	230.04	133.29	131.58	132.32
	231.01	230.90	230.58	134.18	133.19	133.37
	231.50	231.64	230.68	134.66	134.17	134.13
	231.79	231.90	231.12	134.87	134.42	134.61
	232.25	232.18	231.76	134.95	134.83	134.83
	233.12	233.40	232.13	135.01	134.96	134.98
	233.50	233.70	233.02	135.46	135.00	135.25
	237.88	237.90	233.61	135.60	135.39	135.59
	238.11	238.01	237.44	136.03	135.63	135.87
	239.11	239.24	237.65	136.46	135.78	136.02
	239.24	239.44	238.75	136.92	136.22	136.27
	239.76	239.76	238.79	137.32	137.08	137.37
	239.98	239.97	239.40	138.47	137.75	137.61
	240.41	240.50	239.82	138.84	138.50	138.51
	242.17	243.01	240.29	139.12	138.72	138.74
	243.89	245.21	243.74	139.59	139.13	139.16
	450.08	280.62	245.58	139.71	139.40	139.34
	508.33	439.23	360.75	140.80	139.77	139.84
	932.76	513.95	511.57	140.94	140.65	140.60
	3610.11	3591.73	3516.81	141.47	140.87	140.85
Cu/Cu(553)	11.42	-1271.07	11.16	141.66	141.21	141.00
	23.15	11.07	23.34	142.31	141.63	141.35
	30.85	24.67	31.10	143.25	142.29	142.18
	38.93	30.33	36.10	143.47	143.24	143.23
	43.31	32.83	38.87	144.98	143.32	143.34
	46.51	39.22	43.88	145.32	144.93	144.74
	47.45	43.78	46.18	145.65	145.32	145.51
	51.87	47.12	47.62	146.02	145.42	145.57
	52.14	47.78	51.60	146.03	145.76	145.71
	55.09	52.16	52.30	146.21	146.08	145.85
	57.77	52.53	55.24	146.57	146.10	146.10
	58.22	56.24	57.99	147.04	146.40	146.14
	63.65	58.24	58.34	147.28	146.89	146.72
	65.05	58.64	64.02	147.36	147.28	147.00

65.14	64.48	65.07	147.70	147.36	147.30
65.41	65.19	65.13	147.86	147.52	147.42
67.61	65.50	65.41	148.01	147.85	147.81
68.12	65.65	67.91	148.47	148.00	148.03
68.75	68.15	68.58	148.58	148.49	148.50
69.44	69.15	69.26	148.95	148.69	148.54
69.60	69.22	69.67	149.31	149.03	148.96
70.12	70.08	69.98	149.55	149.27	149.11
71.38	70.13	70.27	149.87	149.44	149.60
72.68	70.54	71.53	150.00	149.86	149.76
75.00	71.52	73.17	150.65	149.96	150.05
75.68	73.52	75.54	151.00	150.61	150.41
75.94	76.16	75.96	151.57	150.85	150.82
76.13	76.21	76.19	151.98	151.41	151.49
79.65	76.34	76.46	152.21	151.86	151.86
80.73	76.36	79.91	152.34	152.11	151.99
81.24	80.17	80.65	152.65	152.38	152.25
82.78	81.73	81.76	152.95	152.59	152.48
83.98	81.97	82.72	152.99	152.86	152.76
84.24	84.39	84.46	153.68	153.19	153.01
85.63	84.54	84.47	153.98	153.61	153.53
85.94	84.65	85.82	155.31	153.83	153.82
86.05	86.77	86.56	156.04	155.04	155.63
90.68	86.90	87.18	156.81	155.62	155.72
90.96	87.00	89.34	156.95	156.58	156.72
91.88	91.47	90.84	157.39	157.02	156.96
92.74	92.55	92.54	157.54	157.48	157.10
93.56	92.60	92.87	157.72	157.59	157.45
93.81	93.65	93.96	158.06	157.73	157.80
94.28	94.26	94.18	158.59	158.15	158.03
94.76	94.39	94.28	158.89	158.54	158.56
95.42	94.85	94.89	159.43	158.72	158.84
95.66	94.92	95.11	159.59	159.39	159.38
96.06	95.15	95.43	160.03	159.71	159.66
96.25	95.68	95.78	160.26	160.07	159.98
96.81	96.70	96.41	160.59	160.27	160.18
97.04	97.11	96.96	160.74	160.49	160.24
97.43	97.23	97.98	161.01	160.75	160.70
98.81	97.99	98.05	161.36	160.93	160.89
98.96	98.54	98.49	161.51	161.27	161.41
99.07	99.27	99.18	162.01	161.66	161.96
99.74	99.38	99.36	162.34	161.99	162.26
99.92	99.47	99.55	163.21	162.23	162.29
100.12	99.72	99.79	163.56	163.09	162.95

100.22	99.85	100.09	164.56	163.49	163.51
100.54	100.04	100.49	164.74	164.44	164.42
101.31	100.88	100.79	165.18	164.66	164.59
101.58	101.02	101.41	165.89	164.95	164.88
101.65	101.68	101.61	166.17	165.86	165.71
102.06	101.84	101.80	166.39	166.16	165.94
102.37	102.22	102.61	166.45	166.42	166.45
105.33	102.40	102.76	167.11	166.52	166.46
106.83	102.87	103.66	167.35	167.17	167.05
107.01	106.27	105.59	167.78	167.28	167.33
107.30	107.51	107.34	169.25	167.71	167.72
107.41	107.60	107.46	169.50	169.24	169.23
107.93	107.69	107.59	169.98	169.52	169.67
108.44	108.19	108.16	170.86	169.94	169.83
108.50	108.66	108.42	172.14	170.75	170.74
109.40	109.10	109.04	173.00	172.10	172.08
109.45	109.21	109.14	173.56	172.75	172.96
109.68	109.43	109.74	173.82	173.58	173.54
110.62	109.90	109.89	175.30	173.87	173.80
111.07	110.21	110.34	175.57	174.97	174.94
112.21	110.76	110.98	176.56	175.63	175.63
112.81	111.10	111.14	176.99	176.43	176.33
113.18	113.23	113.40	177.36	176.95	176.88
113.69	113.51	113.63	177.78	177.33	177.19
113.82	113.78	113.96	178.54	177.63	177.44
113.91	114.01	114.12	180.11	178.41	178.40
114.16	114.46	114.22	180.58	179.96	179.78
114.24	114.57	114.31	182.52	180.39	180.41
114.49	114.63	114.36	183.50	182.33	182.40
114.76	114.81	114.57	183.53	183.26	183.09
115.79	114.96	114.92	183.87	183.41	183.33
117.01	115.28	115.04	184.69	183.72	183.86
117.23	115.44	116.12	184.89	184.36	184.13
117.44	117.68	117.45	185.09	184.71	184.68
117.78	117.73	117.56	185.48	185.13	184.97
118.08	117.75	117.67	185.61	185.36	185.19
118.34	118.02	117.83	188.06	185.41	185.32
118.75	119.05	118.49	188.33	187.89	187.55
119.49	119.49	119.25	189.00	188.18	187.79
119.63	119.58	119.37	189.22	188.93	188.80
120.00	119.72	119.51	189.61	189.05	189.06
120.12	119.78	119.61	189.97	189.46	189.49
120.61	120.05	119.84	190.60	190.15	189.98
120.87	120.56	120.36	190.87	190.23	190.22

121.28	120.60	120.50	191.77	190.83	190.73
121.35	121.01	120.79	192.02	191.55	191.47
121.63	121.33	121.14	192.39	191.89	191.61
121.78	121.65	121.51	193.15	191.93	191.80
122.01	121.67	121.63	193.94	192.98	193.06
122.27	122.24	122.24	194.02	193.77	193.66
123.82	122.39	122.30	196.69	194.01	193.81
124.86	122.78	122.79	197.06	196.35	196.24
125.34	124.88	124.94	197.65	196.92	196.62
125.92	125.33	125.47	198.62	197.59	197.48
126.07	125.93	125.82	200.39	198.46	198.31
126.38	126.29	126.25	202.22	200.34	200.53
126.87	126.65	126.43	202.42	202.16	201.94
127.38	126.85	126.75	202.84	202.33	202.14
127.66	127.14	126.93	203.07	202.58	202.33
129.03	127.46	127.46	203.14	202.84	202.76
129.58	127.66	127.60	203.52	203.12	202.91
129.85	129.65	129.45	203.99	203.44	203.39
130.34	129.85	129.61	204.21	204.02	203.90
131.06	129.94	129.93	204.79	204.10	204.03
132.08	130.29	130.25	205.22	204.77	204.72
132.33	131.20	131.14	207.57	205.40	205.02
132.63	132.00	132.08	210.38	207.44	207.64
132.78	132.62	132.28	210.61	210.13	210.24
132.84	132.68	132.48	210.66	210.52	210.60
133.04	132.75	132.70	211.64	210.60	210.71
133.41	132.90	132.74	211.84	211.20	211.23
133.73	133.17	132.85	212.21	212.06	211.69
134.14	133.33	132.88	212.80	212.19	211.93
134.64	134.07	133.70	214.44	212.32	212.11
135.64	134.38	133.84	214.91	214.26	214.03
135.77	134.52	134.33	215.18	214.84	214.78
137.07	135.49	135.35	215.39	215.16	214.98
137.19	136.03	135.81	216.78	215.30	215.15
137.62	137.16	136.91	218.56	216.82	216.69
137.75	137.24	137.29	219.85	218.63	218.43
137.82	137.81	137.57	220.26	219.63	219.42
138.24	137.89	137.70	223.48	220.12	219.86
138.38	138.34	138.14	223.77	223.26	222.98
139.02	138.47	138.25	224.53	223.59	223.14
139.81	138.58	138.56	224.92	224.45	224.29
140.00	139.20	138.91	225.33	224.76	224.39
140.05	139.61	139.59	225.63	225.17	225.03
140.18	139.90	139.79	226.43	225.36	225.18

140.27	139.94	139.83	227.19	225.94	225.65
140.37	140.25	139.93	227.58	226.47	226.33
140.50	140.38	140.02	228.12	227.67	227.58
140.63	140.49	140.30	228.97	228.01	228.26
142.30	140.87	140.62	231.96	229.02	228.66
142.50	141.38	140.99	233.11	231.56	231.38
144.10	142.66	142.32	233.48	232.97	232.65
144.19	142.72	142.49	233.84	233.25	232.98
144.31	143.20	143.31	234.92	233.97	233.57
144.51	144.48	144.27	235.80	234.64	234.23
144.62	144.63	144.37	238.33	235.54	235.20
144.79	144.82	144.41	239.19	238.11	238.12
145.05	144.89	144.64	240.40	238.82	238.55
145.43	145.11	144.74	241.32	240.08	239.83
145.59	145.16	145.13	241.95	241.09	240.86
145.68	145.54	145.24	244.94	241.93	241.76
145.77	145.73	145.56	245.88	244.40	244.20
146.21	145.75	145.76	246.44	245.72	245.47
147.01	145.99	145.82	247.08	246.33	246.04
147.16	146.34	146.09	247.48	246.98	246.37
148.12	147.21	147.04	249.10	247.27	246.90
148.36	147.29	147.27	249.19	249.09	248.73
148.57	148.05	148.02	249.56	249.13	248.80
149.76	148.28	148.16	249.68	249.62	249.44
149.93	148.38	148.51	250.27	249.72	249.62
150.08	149.85	149.56	250.66	250.44	249.99
150.33	150.37	150.16	250.97	250.56	250.16
150.62	150.49	150.26	251.23	251.12	250.69
150.91	150.81	150.44	251.52	251.25	251.11
151.34	150.85	150.74	252.49	251.42	251.12
151.69	151.09	151.06	252.58	252.22	251.79
152.23	151.35	151.22	252.64	252.67	252.18
153.36	152.04	151.85	253.66	252.75	252.34
153.48	152.12	152.16	253.79	253.50	252.99
153.98	153.10	153.11	254.56	253.67	253.18
154.63	153.17	153.17	255.43	254.20	254.03
154.88	154.48	154.04	256.32	255.32	254.84
154.97	154.52	154.20	256.36	256.30	256.07
155.32	154.82	154.87	256.66	256.34	256.10
155.72	154.98	155.16	257.34	256.63	256.16
156.23	155.66	155.44	257.64	257.23	256.79
156.75	155.70	155.65	258.38	257.61	257.20
157.19	156.68	155.81	259.90	258.44	258.10
157.75	156.77	157.25	265.12	259.76	259.30

157.99	157.54	157.40		265.65	265.06	264.78
158.22	157.76	157.53		435.85	265.57	265.37
158.29	157.80	157.65		603.96	308.13	377.77
158.58	158.11	158.03		953.67	346.88	501.30
158.63	158.26	158.20		3575.84	3580.52	3530.58
158.69	158.46	158.25	Zn/Cu(553)	11.03	-1761.85	11.02
158.85	158.54	158.50		23.26	11.26	23.88
159.44	158.67	158.54		31.03	23.36	31.35
160.83	158.88	158.69		39.05	31.22	32.99
161.33	159.66	159.08		43.78	38.97	39.23
161.73	160.12	159.92		46.41	43.52	43.97
161.99	161.39	161.28		47.58	46.07	46.17
162.72	161.64	161.50		51.78	47.38	47.62
163.33	161.89	161.95		52.07	49.14	49.03
164.67	162.45	162.25		54.87	51.85	51.74
164.71	163.13	162.76		57.74	53.57	54.18
165.34	164.69	164.51		58.06	56.86	56.13
165.63	164.85	164.78		63.91	58.00	57.92
166.10	165.70	165.47		65.13	58.27	60.23
166.24	165.81	165.66		65.26	64.64	64.73
167.35	165.93	165.82		65.41	65.21	65.11
169.18	166.14	165.90		67.43	65.31	65.19
169.43	166.84	166.70		67.79	65.52	65.71
169.58	169.05	168.34		68.52	67.42	67.51
169.98	169.33	169.02		69.36	68.61	68.69
171.31	169.59	169.18		69.47	69.21	69.17
171.89	169.85	169.48		70.15	69.41	69.59
173.60	170.88	169.84		71.18	69.77	69.85
173.85	171.42	171.19		72.51	70.39	70.20
174.19	172.62	172.02		74.57	71.07	71.15
174.37	173.69	173.58		75.64	73.33	73.28
174.98	174.12	173.92		76.15	75.30	75.71
175.54	174.35	174.07		76.30	75.80	75.80
175.74	174.54	174.23		79.54	76.23	76.18
176.15	175.06	174.55		80.42	76.36	76.26
177.32	175.63	175.14		81.03	79.25	79.59
177.75	176.02	175.41		82.49	80.99	81.27
179.92	176.46	175.81		83.71	81.10	81.68
180.29	177.71	177.39		84.09	83.70	83.48
180.47	178.04	177.43		85.50	84.12	84.12
180.59	179.61	179.77		85.91	84.29	84.37
181.14	180.39	180.02		86.02	85.95	86.21
181.29	180.57	180.10		90.67	86.33	86.50
182.47	180.71	180.50		90.89	86.75	86.63

182.96	180.87	181.10	91.35	90.93	90.65
183.07	181.41	181.35	92.56	91.09	91.31
183.37	182.80	182.65	93.56	91.42	91.95
184.68	182.97	182.81	93.64	92.26	92.94
184.88	183.33	182.94	94.27	93.67	93.57
186.46	183.64	182.96	94.67	93.94	93.91
187.81	184.84	184.55	94.93	94.06	94.38
188.52	185.12	184.71	95.39	94.52	94.71
189.11	186.36	186.26	95.72	94.86	94.93
189.28	186.92	187.24	96.43	95.32	95.36
189.37	187.73	187.94	96.68	95.61	95.60
189.83	188.95	188.99	97.00	96.43	96.34
190.14	189.22	189.03	97.50	96.83	96.95
191.51	189.28	189.45	98.77	97.40	97.50
191.82	189.65	189.64	99.12	98.21	97.87
192.11	189.94	189.79	99.39	98.51	98.77
193.16	190.69	191.33	99.57	99.10	98.84
193.72	191.79	191.74	99.88	99.22	99.25
197.09	191.92	192.00	100.13	99.34	99.40
197.79	192.37	193.21	100.34	99.42	99.60
199.42	193.73	193.28	100.51	100.10	99.85
199.89	193.83	196.93	101.26	100.43	100.02
200.96	197.18	197.44	101.48	100.81	100.59
201.74	198.97	199.28	101.86	101.34	100.75
202.34	199.81	199.65	102.20	101.55	101.43
203.88	199.87	200.94	102.65	101.73	101.69
204.11	201.23	201.58	105.15	102.19	102.31
204.74	201.81	202.09	105.90	102.49	102.59
204.81	202.34	204.09	107.11	106.00	102.96
205.17	204.53	204.23	107.21	107.31	105.52
205.47	204.67	204.42	107.47	107.42	107.41
206.47	204.81	204.53	107.95	107.59	107.49
208.05	205.00	204.79	108.61	107.97	107.79
208.12	205.11	204.86	109.06	108.30	108.27
209.15	205.41	206.43	109.30	108.45	108.39
209.71	206.67	207.84	109.41	108.88	108.76
210.95	208.36	208.09	109.89	109.18	109.06
211.48	208.46	209.28	110.22	109.29	109.42
211.88	209.72	209.72	111.22	109.94	109.71
212.34	209.90	210.85	112.03	110.14	109.99
212.97	211.32	211.17	112.65	110.78	110.81
213.89	211.57	211.47	113.33	112.40	111.04
213.96	212.11	211.88	113.57	112.62	112.77
215.42	212.26	212.25	113.68	113.24	113.35

215.57	213.52	213.74	113.95	113.49	113.53
215.79	213.96	214.00	114.02	113.94	113.67
217.18	214.60	215.27	114.29	114.03	114.02
218.55	215.74	215.36	114.41	114.19	114.17
218.75	215.79	215.65	114.89	114.27	114.31
220.06	216.09	216.95	115.36	114.52	114.42
220.43	217.25	218.31	116.31	114.64	114.57
220.60	218.87	218.45	117.40	114.94	114.85
221.69	218.96	219.92	117.48	116.41	114.99
222.18	220.50	220.05	117.67	117.05	116.43
224.65	220.53	220.60	117.83	117.57	117.24
225.10	221.08	221.66	118.22	117.71	117.62
225.76	222.11	221.77	118.77	117.99	117.68
226.32	222.52	224.12	119.29	118.76	117.93
228.49	224.57	224.93	119.67	119.05	118.52
229.51	225.00	225.58	119.82	119.22	119.27
229.78	225.74	226.07	120.13	119.54	119.35
229.96	226.22	228.57	120.46	119.76	119.58
230.47	228.94	229.15	120.85	120.09	119.65
232.60	229.65	229.38	121.06	120.41	119.98
235.57	230.02	229.77	121.13	120.87	120.42
236.14	230.20	230.05	121.46	120.95	120.64
236.33	230.56	231.81	121.88	121.15	120.97
237.63	232.06	235.08	121.89	121.27	121.34
237.81	235.62	235.55	122.27	121.88	121.50
240.83	235.99	236.12	123.65	121.97	121.73
240.89	236.55	237.61	124.98	122.36	122.09
241.91	237.95	237.71	125.43	123.99	122.33
242.20	238.09	240.55	125.66	124.68	124.36
244.70	240.93	240.77	125.78	125.12	124.96
245.18	241.22	241.52	126.40	125.96	125.23
245.34	241.96	241.95	126.87	126.06	125.89
245.54	242.50	243.20	127.20	126.32	126.23
246.07	244.95	245.04	127.79	126.78	126.48
246.27	245.49	245.09	128.61	127.10	126.64
246.50	245.56	245.36	129.38	127.46	127.18
246.54	245.66	245.59	129.54	128.65	127.56
246.72	246.24	245.99	130.14	129.09	128.66
246.86	246.45	246.07	130.83	129.43	129.13
246.99	246.53	246.18	131.90	129.87	129.57
247.34	246.59	246.25	132.18	130.83	129.89
247.70	246.73	246.63	132.50	131.39	130.58
248.00	247.03	246.82	132.80	132.27	131.08
248.73	247.12	246.87	132.93	132.46	132.16

	249.38	247.21	246.97	133.06	132.67	132.28
	250.82	247.28	247.27	133.43	132.96	132.47
	251.85	247.56	247.37	133.63	133.00	132.81
	251.95	247.65	248.65	134.08	133.17	132.86
	252.04	249.20	250.29	134.75	133.99	133.12
	252.42	250.72	250.53	135.38	134.05	133.66
	253.06	251.38	251.92	135.95	134.66	133.83
	255.77	252.14	251.94	136.62	135.25	134.38
	257.01	252.21	252.56	137.15	135.37	135.11
	261.07	252.25	252.72	137.56	136.38	135.60
	262.38	252.99	255.15	137.80	137.07	136.66
	384.98	255.62	256.65	137.84	137.34	137.10
	437.73	256.98	259.60	138.12	137.62	137.42
	525.06	260.56	261.47	138.25	137.71	137.48
	547.99	261.89	283.70	138.90	137.98	137.65
	557.50	390.07	503.37	139.31	138.43	137.81
	3559.11	1669.03	3547.94	139.72	139.00	138.38
Nb/Cu(553)	12.13	-1203.21	10.00	139.88	139.16	138.67
	16.63	11.65	15.14	140.08	139.35	138.90
	21.85	21.50	22.35	140.15	139.85	139.32
	31.67	31.60	31.72	140.28	140.04	139.68
	38.15	36.70	38.56	140.49	140.18	139.88
	42.45	38.08	42.83	140.68	140.28	139.99
	44.74	38.69	43.18	142.02	140.43	140.11
	46.34	43.62	45.20	142.33	141.08	140.11
	52.41	45.02	52.60	142.74	141.94	140.77
	53.75	52.19	53.72	143.96	142.04	141.87
	54.72	53.79	54.94	144.22	142.61	142.34
	58.77	54.20	58.85	144.36	144.29	142.39
	59.66	58.56	59.75	144.54	144.51	144.19
	60.89	59.68	60.72	144.74	144.56	144.32
	63.53	60.03	63.39	144.82	144.62	144.39
	65.05	63.13	64.79	145.31	144.83	144.48
	66.37	64.95	67.10	145.60	144.93	144.57
	67.25	66.79	67.29	145.62	145.21	144.62
	67.49	67.19	68.07	145.80	145.74	145.18
	69.26	67.87	69.09	146.29	145.83	145.41
	69.66	69.57	69.83	146.96	145.86	145.62
	69.95	69.88	70.14	147.41	146.26	145.95
	70.54	70.18	70.30	147.87	147.11	146.12
	71.20	70.40	71.23	148.32	147.45	146.97
	73.13	71.29	73.21	148.39	147.75	147.20
	76.06	73.13	75.96	149.51	148.23	147.81
	76.48	76.01	76.61	149.71	148.35	148.12

77.28	76.64	77.18	149.99	149.42	148.28
77.48	77.35	77.33	150.45	149.61	149.46
77.78	77.47	77.40	150.47	149.81	149.61
78.99	77.76	78.91	150.82	150.21	149.94
81.90	78.96	82.01	151.35	150.60	150.07
82.63	82.03	82.41	151.83	150.82	150.35
84.17	82.63	84.05	152.31	151.21	150.68
84.29	84.08	84.13	153.21	151.77	151.04
85.14	84.30	85.37	153.51	152.29	151.57
85.75	85.25	85.79	153.99	152.87	152.32
86.24	85.78	86.27	154.50	153.12	152.75
87.32	86.34	86.98	154.68	154.12	152.95
88.86	87.23	89.69	154.90	154.40	153.93
91.92	89.59	92.14	155.12	154.69	154.32
93.06	92.27	92.89	155.76	154.98	154.73
93.53	92.84	93.84	156.21	155.03	154.98
93.92	93.87	94.27	156.55	155.63	155.40
94.25	94.16	94.60	157.21	156.34	155.51
94.76	94.71	95.07	157.70	156.44	156.21
95.96	94.82	95.49	157.88	157.33	156.92
96.57	95.67	96.54	158.07	157.56	157.30
96.80	96.67	96.67	158.31	157.61	157.52
96.82	96.84	96.88	158.50	157.95	157.59
97.87	96.98	98.63	158.61	158.05	157.75
98.28	98.38	98.91	158.82	158.20	157.95
99.10	98.50	99.31	158.83	158.42	158.14
99.51	99.24	99.92	159.96	158.65	158.26
99.66	99.83	100.13	160.57	158.83	158.50
99.79	99.92	100.46	161.10	159.72	158.67
100.66	100.37	100.50	161.67	159.78	159.27
100.81	100.69	100.69	162.05	161.10	159.88
100.89	100.86	100.98	162.56	161.69	160.96
101.02	100.93	101.04	163.01	162.03	161.56
101.45	100.97	101.45	164.65	162.32	161.70
101.51	101.53	101.72	164.77	162.93	162.09
101.73	101.77	101.85	164.84	164.71	162.41
101.88	101.82	102.29	165.65	164.84	164.47
102.34	102.11	102.70	165.91	164.86	164.61
103.07	102.52	103.55	166.22	165.47	164.86
103.64	103.40	104.10	167.31	165.77	165.39
106.10	103.59	106.40	168.91	166.04	165.61
106.20	106.26	106.45	169.19	166.91	165.89
106.55	106.32	106.87	169.58	168.90	166.72
107.17	106.73	107.65	169.92	169.20	168.60

107.61	107.34	107.73	171.23	169.57	168.95
107.94	107.39	108.76	172.26	169.81	169.41
108.98	108.46	109.06	173.42	171.20	169.59
110.59	108.52	110.02	173.69	171.97	171.14
110.89	110.34	110.75	173.98	173.31	172.04
111.07	110.86	111.32	174.34	173.55	173.11
111.67	111.19	111.64	174.63	173.80	173.47
112.51	111.59	112.54	175.25	174.29	173.80
113.00	112.72	113.15	175.73	174.69	174.04
113.39	113.01	113.26	175.87	175.34	174.52
113.65	113.35	113.82	177.17	175.52	175.11
113.79	113.63	113.89	177.65	175.88	175.22
114.69	113.75	114.87	179.30	177.31	175.68
114.83	114.67	115.04	180.09	177.62	177.22
115.28	114.91	115.18	180.43	179.67	177.46
115.43	115.18	115.32	180.68	180.06	179.31
115.62	115.31	115.39	180.85	180.31	179.79
116.56	115.46	115.94	181.29	180.51	179.91
116.81	116.14	116.56	182.39	181.00	180.18
117.77	116.57	117.19	182.64	181.33	180.73
117.99	117.71	117.84	183.12	182.13	181.23
118.15	117.92	118.08	183.15	182.83	182.01
119.25	118.37	118.94	184.26	183.01	182.48
119.60	119.19	119.19	184.43	183.13	182.75
120.00	119.46	119.52	185.87	184.31	182.86
121.44	119.77	121.31	187.68	184.68	184.13
121.48	121.42	121.45	188.15	185.74	184.46
121.63	121.54	121.66	188.59	187.51	185.45
122.03	121.68	121.96	189.14	188.30	186.72
122.51	121.98	122.35	189.54	188.66	188.02
122.77	122.44	122.55	189.63	188.97	188.54
122.87	122.77	122.69	190.21	189.27	188.90
122.93	122.84	122.94	191.35	189.80	189.19
123.30	122.98	123.03	191.64	190.17	189.68
123.46	123.20	123.41	192.05	191.28	190.13
123.85	123.43	123.62	192.72	191.72	191.10
123.88	123.75	123.79	193.41	192.10	191.62
124.43	123.83	124.19	197.11	193.12	192.07
124.73	124.30	124.54	198.13	193.28	192.85
125.37	124.61	125.08	199.20	197.09	193.13
125.53	125.39	125.51	199.68	197.56	196.96
125.99	125.45	125.92	200.62	199.15	197.51
126.52	126.32	126.47	201.74	199.98	198.72
127.85	126.55	127.95	202.28	200.74	199.57

128.15	127.94	128.01	203.38	201.72	200.56
128.65	128.00	128.40	203.58	202.19	201.53
129.10	128.53	128.87	204.54	203.38	202.05
129.22	128.74	129.29	204.73	203.68	203.31
129.50	129.36	129.64	205.34	204.34	203.92
130.39	129.63	129.94	205.74	204.72	204.24
131.08	130.21	130.56	206.01	204.98	204.53
131.43	130.89	131.01	207.79	205.30	204.74
132.31	131.18	132.16	207.94	206.21	205.02
133.56	132.09	133.56	209.07	207.88	205.91
133.91	133.52	133.94	209.39	208.15	207.54
134.38	134.00	134.37	210.53	209.24	207.94
134.73	134.37	134.68	211.13	209.73	209.01
134.91	134.76	134.82	211.90	210.35	209.39
135.03	134.99	134.94	212.16	211.31	209.54
135.48	135.02	135.69	212.91	211.64	211.05
135.80	135.70	135.81	213.84	212.12	211.24
136.01	135.89	136.33	214.04	212.44	211.95
136.91	136.27	136.99	215.37	213.17	212.47
137.35	136.77	137.37	215.74	213.94	213.70
138.34	137.08	138.45	215.82	214.70	213.99
138.75	138.37	138.58	217.05	215.69	215.16
138.97	138.62	138.76	218.56	215.95	215.41
139.41	138.85	139.19	218.80	216.93	215.80
139.54	139.21	139.38	220.10	218.20	216.79
140.24	139.48	140.00	220.42	218.50	218.11
140.76	140.21	140.59	220.71	219.05	218.59
141.45	140.71	140.94	221.43	220.28	219.82
141.48	141.16	141.26	222.30	220.49	220.06
141.76	141.44	141.41	223.56	221.05	220.67
142.50	141.65	142.09	224.54	222.01	221.77
143.12	142.35	143.00	225.68	222.11	221.79
143.74	143.16	143.45	225.78	223.56	222.18
145.37	143.55	145.25	228.54	224.83	224.57
145.46	145.38	145.33	228.78	225.71	225.49
145.79	145.44	145.44	229.69	225.98	225.77
145.97	145.63	145.63	229.99	228.59	227.42
146.20	145.88	145.77	230.32	229.10	228.64
146.21	146.23	146.07	231.39	229.97	229.50
146.43	146.28	146.21	233.83	230.17	229.86
146.96	146.35	146.72	235.76	230.37	229.94
147.39	146.92	147.13	236.04	231.95	231.36
147.57	147.44	147.21	236.63	234.57	233.97
147.78	147.49	147.45	237.93	236.07	235.68

148.04	147.68	147.73		239.65	236.40	235.75
148.14	147.89	148.01		240.85	236.91	236.68
148.31	148.14	148.13		241.71	238.05	237.84
148.50	148.41	148.43		242.04	240.01	238.99
148.82	148.58	148.80		243.05	241.23	240.83
149.47	149.07	149.05		244.94	241.39	240.93
149.75	149.38	149.42		245.28	242.70	241.91
149.83	149.65	149.76		245.50	243.20	242.24
150.25	149.88	150.08		246.02	245.62	245.04
150.61	150.10	150.45		246.13	245.63	245.09
150.94	150.63	150.66		246.30	245.89	245.47
151.88	150.80	151.66		246.59	246.05	245.55
152.18	151.90	151.87		246.65	246.49	246.09
152.23	152.21	152.04		247.04	246.57	246.17
152.60	152.28	152.21		247.11	246.66	246.25
152.73	152.53	152.61		247.45	246.71	246.32
152.92	152.77	152.69		247.83	247.46	246.69
153.09	152.81	152.89		248.19	247.53	246.74
154.44	153.24	153.85		249.00	247.64	246.95
154.81	154.10	154.15		249.44	247.75	247.16
155.34	154.50	155.12		250.69	248.01	247.35
156.06	155.23	155.30		250.92	248.36	247.40
156.97	155.46	156.51		252.04	249.41	248.60
157.18	156.89	157.02		252.16	250.87	249.56
157.42	157.18	157.21		252.25	251.15	250.39
157.65	157.50	157.37		252.96	252.12	252.00
157.96	157.54	157.72		255.84	252.13	252.01
158.11	158.03	157.88		257.15	253.21	252.47
158.70	158.27	158.30		261.15	254.20	252.77
159.23	158.62	158.96		262.18	255.86	255.23
159.71	158.97	159.52		366.34	257.17	256.56
159.86	159.82	159.69		450.30	261.09	257.60
159.90	159.92	159.87		538.52	262.38	261.30
160.22	160.02	160.01		554.49	469.24	264.01
160.41	160.17	160.12		603.37	549.86	432.37
160.89	160.39	160.75		3548.09	3496.97	3537.93
161.19	160.96	161.03	Cd/Cu(553)	20.68	-1679.23	21.31
161.77	161.36	161.41		30.71	20.81	32.63
162.04	161.54	161.70		35.53	32.24	38.46
162.20	161.84	162.07		40.48	38.17	43.69
162.44	162.11	162.18		43.60	43.06	44.98
163.39	162.45	162.88		45.31	44.36	52.26
164.05	163.45	163.45		52.28	46.46	53.59
164.57	164.08	163.92		53.65	52.64	54.09

164.78	164.56	164.48	54.45	53.53	59.07
165.71	164.92	164.87	58.98	53.88	59.74
165.91	165.29	165.22	59.85	59.08	60.00
166.24	166.11	165.86	61.23	59.95	64.20
166.38	166.35	166.19	64.26	60.03	64.83
166.72	166.45	166.23	65.02	64.33	65.16
167.38	166.56	166.43	65.89	64.88	67.34
167.49	167.26	167.05	67.27	65.07	67.61
167.83	167.72	167.64	67.73	67.06	69.46
169.43	168.23	167.90	69.70	67.29	70.53
169.80	169.47	169.38	70.49	69.45	71.07
170.90	169.79	169.71	71.26	70.25	71.62
171.58	170.90	170.80	71.50	70.77	71.73
172.19	171.74	171.44	72.81	71.59	74.79
173.28	172.07	171.91	74.62	71.74	75.36
173.67	173.28	173.18	76.32	74.79	77.09
174.27	173.65	173.48	77.00	75.37	78.06
175.78	174.61	174.40	78.27	76.80	78.48
175.90	175.50	175.24	78.67	78.14	79.03
176.75	176.07	176.08	78.88	78.40	79.17
177.20	176.76	176.51	80.78	78.81	82.63
177.96	177.22	176.98	83.00	79.08	83.61
178.56	177.89	177.70	83.32	82.10	84.03
178.74	178.25	178.08	83.65	83.23	84.55
180.59	178.68	178.57	84.50	83.58	86.09
180.75	180.39	180.08	85.04	84.21	86.36
183.19	180.68	180.55	86.33	85.72	86.79
183.64	183.15	182.83	87.41	86.36	88.32
183.69	183.57	183.34	88.03	86.53	88.45
183.95	183.69	183.43	89.48	87.18	90.94
185.00	183.90	183.85	90.01	88.46	91.69
185.20	184.91	184.71	92.00	89.04	93.18
185.61	185.22	184.98	93.56	91.67	93.58
186.47	185.46	185.21	94.00	92.14	94.66
186.68	186.24	185.73	94.49	93.02	95.38
187.89	186.52	186.12	94.93	94.38	95.78
188.53	187.82	187.57	95.74	94.46	96.30
189.39	188.40	188.06	96.49	95.38	97.13
189.54	189.44	189.28	96.91	96.19	97.82
189.85	189.62	189.53	97.57	96.77	98.67
190.35	190.07	189.85	98.40	97.55	98.89
190.97	190.23	189.90	98.75	98.31	99.11
191.08	190.77	190.50	99.16	98.40	99.45
191.83	190.97	190.81	99.55	98.90	99.79

192.07	191.75	191.50	99.73	99.39	100.18
192.60	192.00	191.63	99.93	99.52	100.88
193.43	192.46	192.11	100.10	100.01	100.95
194.05	193.57	193.64	100.96	100.36	101.01
194.29	193.90	193.77	101.05	100.79	101.43
196.76	194.09	193.88	101.46	100.94	101.90
197.09	196.60	196.40	102.07	101.10	102.28
197.68	197.03	196.73	102.43	101.49	102.32
199.81	197.65	197.49	102.53	101.92	102.74
200.81	199.51	199.46	102.77	102.19	102.82
202.31	200.93	200.72	103.09	102.61	103.03
202.48	202.27	201.96	104.08	102.66	104.66
202.93	202.52	202.19	105.22	102.94	105.60
203.12	202.85	202.57	105.63	104.59	105.95
203.72	203.08	202.71	106.29	105.21	106.50
203.83	203.74	203.41	106.57	105.71	106.54
204.26	203.79	203.50	106.86	106.18	107.37
205.16	204.36	204.19	107.40	106.77	108.30
205.99	205.34	205.03	109.06	106.86	109.50
206.28	205.68	205.59	109.20	107.78	109.84
207.79	205.99	205.63	109.61	108.93	110.84
210.57	207.85	207.69	110.66	109.33	111.27
210.71	210.56	210.42	111.84	109.54	112.04
211.26	210.76	210.60	112.48	110.64	112.92
211.55	211.31	211.13	112.76	111.31	113.43
212.16	211.92	211.67	113.52	111.79	113.68
212.96	212.18	211.82	113.86	112.80	114.37
214.97	212.49	212.40	114.34	112.94	114.45
215.18	214.96	214.75	114.63	113.80	114.77
215.68	215.06	214.89	114.78	114.10	115.06
216.20	215.47	215.35	115.04	114.34	115.10
216.63	215.95	215.52	115.16	114.63	115.46
218.39	216.42	216.34	115.53	114.82	115.74
219.52	218.01	218.03	115.80	115.18	116.19
220.23	219.11	218.91	116.18	115.45	116.29
221.09	219.97	219.76	116.88	115.54	117.12
223.50	220.19	219.85	118.00	116.16	118.22
223.70	223.34	222.94	118.26	116.36	118.39
224.73	223.45	223.18	119.00	117.30	119.65
224.83	224.67	224.27	119.61	118.19	120.14
225.40	224.72	224.50	120.44	118.30	120.79
225.55	225.30	225.05	121.17	119.64	121.92
226.98	225.38	225.14	121.79	120.07	122.12
227.70	226.65	226.29	122.23	121.48	122.25

227.81	227.78	227.71	122.42	121.58	122.62
229.43	227.82	227.84	122.61	122.09	122.63
229.89	229.53	229.06	122.88	122.15	123.00
232.48	229.79	229.48	122.94	122.50	123.23
233.26	232.51	232.35	123.08	122.62	123.73
234.00	233.15	232.83	123.91	122.95	123.89
234.29	233.88	233.63	124.14	123.13	124.14
234.96	234.28	233.95	124.27	123.46	124.32
235.92	234.65	234.32	124.45	123.64	124.50
238.71	235.64	235.37	125.01	124.04	125.17
240.53	238.62	238.47	125.33	124.20	125.63
241.71	240.43	240.05	125.83	124.33	125.93
242.01	241.10	240.78	126.13	125.10	126.17
243.22	241.95	241.66	126.33	125.55	126.37
245.99	243.28	242.45	126.78	125.99	127.24
246.17	245.80	245.24	127.52	126.25	127.71
246.82	246.13	245.59	127.82	126.35	127.98
247.14	246.71	245.85	128.21	127.37	128.35
248.92	247.10	246.50	129.08	127.66	129.11
249.00	248.76	248.11	129.38	127.91	129.68
249.52	249.07	248.51	129.91	128.36	130.08
249.60	249.54	248.80	130.01	129.09	130.35
249.97	249.67	248.91	130.26	129.72	130.73
250.31	249.99	249.42	131.45	130.14	131.77
250.64	250.30	249.53	132.35	130.27	132.18
250.95	250.57	249.94	132.85	130.73	132.77
251.25	251.08	250.22	133.51	131.56	133.33
251.70	251.29	250.99	133.81	132.48	133.75
252.25	251.89	251.15	134.07	132.79	134.21
252.36	252.11	251.34	134.52	133.34	134.47
253.09	252.64	251.56	135.45	133.91	135.11
253.60	252.83	252.25	136.08	134.15	135.93
253.75	253.49	252.87	136.35	134.56	136.33
255.18	253.63	253.02	136.61	135.30	136.74
256.03	255.01	254.28	137.07	135.90	136.96
256.38	255.88	255.44	137.31	136.24	137.52
256.44	256.36	256.01	137.84	136.68	137.72
256.96	256.41	256.09	138.35	136.75	137.98
257.62	256.80	256.14	138.49	137.63	138.40
258.04	257.49	257.02	138.90	137.81	138.61
258.58	257.58	257.17	139.03	138.17	138.94
259.90	258.45	257.77	139.91	138.51	139.10
265.46	259.73	259.16	140.55	138.72	140.19
266.19	265.45	265.20	141.13	139.08	140.67

	470.49	266.12	265.73	141.32	140.45	140.84
	621.41	332.92	349.42	141.57	140.79	140.99
	879.56	369.77	526.97	142.01	140.96	141.65
	3573.83	3584.38	3535.05	142.41	141.12	142.07
Ta/Cu(553)	19.11	-1861.26	19.01	143.03	141.79	142.58
	22.39	22.37	20.60	143.67	142.14	143.32
	31.79	31.94	22.29	143.99	142.76	143.67
	39.01	39.40	32.05	144.95	143.29	144.09
	44.16	44.74	39.55	145.39	143.84	145.04
	45.44	45.70	43.32	145.93	144.63	145.43
	52.30	52.30	45.76	146.10	145.14	145.96
	53.44	53.36	52.51	146.56	145.33	146.55
	55.64	56.75	53.33	146.71	145.90	146.82
	58.59	58.60	54.84	147.44	146.54	146.87
	59.73	59.54	57.78	147.63	147.03	147.40
	62.50	62.63	58.92	147.79	147.05	147.63
	63.02	62.85	60.15	148.01	147.54	147.66
	64.45	64.54	62.81	148.20	147.77	147.78
	65.49	65.72	64.77	148.36	147.81	147.91
	66.63	66.72	64.86	148.67	148.07	148.34
	67.40	67.44	66.70	148.82	148.18	148.58
	68.64	68.97	67.13	149.18	148.46	148.79
	71.29	71.32	68.51	149.41	148.69	149.34
	71.43	71.45	70.99	149.88	148.78	149.49
	71.46	71.60	71.02	149.91	149.33	149.59
	71.98	72.15	71.46	150.36	149.54	149.84
	73.73	74.08	71.73	150.80	149.72	149.89
	75.70	75.76	72.23	151.24	149.99	151.17
	77.53	77.85	74.34	151.53	150.11	151.49
	78.06	77.94	77.22	152.03	151.18	151.64
	78.48	78.56	77.62	152.07	151.52	151.75
	78.61	78.64	77.86	152.28	151.62	151.95
	82.20	82.33	78.55	152.30	151.93	152.20
	83.17	83.03	79.04	152.93	151.99	152.49
	83.93	83.94	82.32	153.16	152.26	152.72
	84.22	84.34	83.79	153.50	152.47	152.82
	85.03	85.15	84.25	154.60	152.75	153.88
	86.61	86.60	84.53	154.88	152.94	154.70
	87.20	87.22	85.34	155.68	154.17	155.19
	88.19	88.06	86.92	157.00	154.76	155.98
	90.47	91.10	87.15	157.30	155.17	156.73
	91.18	91.39	88.24	157.42	155.80	157.21
	92.20	92.14	91.15	157.80	156.69	157.63
	93.08	93.52	91.39	157.98	157.18	157.78

93.71	94.03	92.58	158.16	157.62	157.90
94.14	94.31	93.73	158.82	157.78	158.93
95.79	95.74	94.10	159.22	158.02	159.08
96.12	96.34	94.64	159.38	158.78	159.14
97.28	97.41	95.87	159.96	158.98	159.19
97.79	98.00	96.73	160.31	159.14	159.81
98.05	98.14	97.30	160.79	159.24	160.22
98.35	98.53	98.14	161.06	159.70	160.62
98.87	98.69	98.26	161.44	160.12	160.66
99.66	99.70	98.66	161.57	160.52	161.04
99.84	99.96	99.21	161.97	160.66	161.29
99.91	100.19	99.87	163.33	161.25	162.06
100.31	100.47	99.89	163.53	161.72	163.17
100.92	100.85	100.18	163.61	162.14	163.55
101.48	101.70	100.47	163.82	163.28	163.63
102.19	102.31	100.89	164.29	163.52	163.85
102.39	102.70	101.91	164.73	163.64	164.10
102.72	102.79	102.16	164.92	163.73	164.69
102.85	103.08	102.50	166.00	164.03	164.76
103.27	103.34	102.75	166.54	164.59	166.01
103.81	103.70	102.94	166.96	164.86	166.74
104.40	104.15	103.39	167.40	165.89	166.95
104.61	104.53	103.59	167.63	166.57	167.09
105.23	105.25	104.14	167.84	166.87	167.30
105.94	105.96	104.42	168.98	167.36	167.52
106.74	106.89	105.27	169.58	167.41	168.47
107.09	107.15	105.97	170.10	167.59	169.21
107.40	107.40	106.49	170.39	168.50	170.58
108.61	108.65	107.09	170.76	169.21	170.66
109.08	108.70	107.27	171.42	170.52	170.94
109.47	109.12	108.35	172.24	170.64	171.81
111.47	111.52	108.75	173.31	170.88	172.93
112.21	112.08	109.45	174.20	171.75	173.25
112.52	112.34	111.53	174.69	172.80	174.36
113.26	113.30	112.15	175.21	173.28	174.65
113.75	113.67	112.47	176.26	174.06	175.16
114.23	113.84	112.85	177.09	174.77	176.73
114.73	114.42	113.72	177.24	175.54	176.93
115.15	115.00	114.14	177.92	176.64	177.46
115.65	115.17	114.52	178.40	176.87	177.75
116.17	115.71	114.80	180.33	177.48	178.46
116.51	116.41	115.50	181.40	177.73	180.04
116.59	116.56	115.95	181.47	178.56	180.59
117.12	117.22	116.23	182.84	180.00	182.47

117.48	117.38	116.31	183.29	180.55	183.05
117.57	117.52	116.72	183.57	182.50	183.21
117.80	117.71	116.95	183.98	183.33	183.35
118.16	117.77	117.19	184.97	183.41	184.46
118.81	118.74	117.32	185.12	183.50	185.03
119.39	118.90	117.76	185.48	184.67	185.17
119.71	119.53	118.40	186.32	185.31	185.34
120.44	120.41	118.88	187.51	185.34	186.24
121.21	121.07	119.41	187.77	185.55	187.63
122.47	122.07	120.26	187.97	186.33	187.77
123.03	122.76	120.95	188.80	187.86	188.71
123.07	122.99	121.60	189.07	188.01	189.08
123.35	123.21	122.40	189.84	188.73	189.16
123.71	123.67	122.70	189.99	189.08	189.83
124.10	123.75	123.16	190.46	189.30	189.98
124.31	123.94	123.46	191.16	189.65	190.34
124.73	124.45	123.55	191.69	189.75	191.26
125.29	124.80	123.97	192.89	190.25	191.41
125.47	125.27	124.46	193.37	191.37	192.77
125.75	125.72	124.59	193.61	191.46	193.36
126.43	125.94	125.23	194.52	192.98	193.78
126.76	126.50	125.39	197.12	193.17	193.92
127.15	126.94	125.59	197.26	193.80	196.79
127.27	127.19	126.38	197.65	194.05	197.14
128.24	127.47	126.66	198.32	196.82	197.24
129.02	128.76	127.12	199.45	197.14	199.28
129.17	129.04	127.37	200.95	197.22	200.97
129.42	129.48	128.53	201.92	199.54	201.86
130.04	129.64	128.91	202.53	200.86	202.16
130.39	129.73	129.02	202.75	201.95	202.58
130.82	130.77	129.26	203.14	202.30	202.82
131.34	131.13	130.53	203.97	202.42	203.06
133.07	131.37	130.77	204.35	203.06	204.14
133.38	132.83	130.85	204.67	203.31	204.34
133.93	133.48	131.56	205.83	204.38	204.96
134.72	133.93	132.31	206.47	204.54	205.54
135.23	134.74	133.25	207.26	204.82	206.26
135.31	135.05	133.46	207.68	205.39	207.38
135.57	135.41	134.70	210.16	206.04	210.05
136.05	135.58	135.15	210.55	207.08	210.81
136.29	136.08	135.37	210.94	210.05	210.90
136.85	136.45	135.78	211.43	210.69	211.47
137.54	136.80	136.04	213.01	210.78	211.84
138.73	137.56	136.72	213.29	211.47	213.28

138.96	138.75	136.91	214.60	211.61	214.61
139.43	139.29	137.32	215.52	213.35	214.93
139.66	139.63	138.88	215.95	214.45	215.60
140.45	140.07	139.02	216.45	214.85	216.00
141.35	140.27	139.23	217.20	215.81	216.62
141.44	141.15	139.70	218.33	215.87	217.39
142.09	141.52	140.04	219.58	216.46	218.20
142.21	142.01	141.31	220.54	217.11	220.03
142.60	142.27	141.56	222.33	217.86	220.98
143.36	142.50	141.92	223.89	220.26	223.80
143.61	142.74	142.15	224.52	221.24	224.36
144.36	144.07	142.55	225.05	223.88	224.57
144.54	144.14	143.46	225.35	224.44	225.22
145.04	144.48	143.62	225.65	224.80	225.72
145.07	145.17	144.24	226.49	225.01	226.29
145.59	145.21	144.44	226.81	225.79	226.45
145.66	145.42	144.94	227.81	226.34	227.44
146.35	145.85	145.10	227.96	226.56	227.59
146.69	145.99	145.57	229.12	227.14	228.68
147.66	146.37	145.77	230.69	227.41	229.21
148.05	147.58	145.99	231.85	229.08	231.25
148.73	148.09	146.79	233.00	229.20	232.46
148.84	148.71	147.97	233.78	231.56	232.64
149.21	148.94	148.59	234.52	232.62	233.39
149.30	149.19	148.78	235.39	232.97	234.17
149.56	149.42	148.93	237.82	233.52	237.53
150.70	149.71	149.13	238.61	234.06	238.10
151.35	150.92	149.35	240.73	237.57	239.76
151.69	151.10	149.59	241.98	238.15	241.39
152.05	151.88	150.66	242.14	239.86	241.75
152.16	152.01	151.43	243.49	241.05	242.15
152.65	152.10	151.87	245.17	241.96	244.79
152.74	152.37	151.90	245.77	242.12	246.11
152.99	152.55	152.04	246.83	245.21	246.72
153.36	153.28	152.16	247.49	246.36	246.99
153.69	153.49	152.97	247.78	246.54	247.46
154.17	153.74	153.09	249.06	247.33	248.97
154.84	154.19	153.27	249.27	247.56	249.08
155.00	154.82	153.94	249.39	249.39	249.98
155.28	155.14	154.24	250.48	249.50	250.25
155.67	155.25	154.85	250.69	249.92	250.87
155.74	155.48	154.97	250.93	250.21	250.94
156.14	155.65	155.40	251.31	250.87	251.20
156.36	155.82	155.46	251.83	251.15	251.56

156.57	156.28	155.73		252.31	251.37	251.87
156.92	156.52	156.01		253.48	251.92	253.23
157.13	156.68	156.17		253.80	252.18	253.75
157.76	157.34	156.44		254.25	253.56	254.06
158.15	157.46	156.88		254.99	254.07	254.59
158.53	157.99	157.18		255.40	254.33	254.95
159.03	158.29	157.69		256.54	254.84	255.67
159.55	158.73	158.02		257.01	255.34	256.62
160.09	159.63	158.38		257.19	256.32	256.73
160.52	159.78	158.92		257.40	256.84	256.88
160.71	160.23	159.18		257.83	256.96	257.74
160.98	160.72	159.84		258.24	257.17	258.02
161.47	161.06	160.69		258.60	258.17	258.39
161.75	161.19	160.90		259.57	258.27	259.42
161.85	161.75	160.94		261.99	258.65	261.55
162.33	161.83	161.60		266.41	259.16	265.51
162.98	162.20	161.72		267.88	261.90	266.45
163.25	163.06	161.93		442.50	266.20	285.97
163.49	163.16	162.43		445.24	267.19	447.27
163.84	163.47	162.98		547.25	386.19	472.83
164.35	164.21	163.19		565.38	642.73	1088.67
164.53	164.51	163.94		3531.71	3438.40	3515.71
164.91	164.57	164.08	W/Cu(553)	11.60	-1125.42	11.42
165.45	164.66	164.42		23.67	23.75	23.90
165.63	165.67	164.48		30.24	30.23	30.11
166.21	165.70	165.32		39.22	39.26	34.04
166.37	166.37	165.57		42.38	42.82	39.70
166.71	166.49	166.17		44.14	44.57	42.24
167.06	166.60	166.31		45.23	45.38	44.69
167.87	167.00	166.60		50.70	50.68	45.26
168.13	167.64	166.65		51.31	51.54	50.63
168.50	168.20	167.38		53.44	53.79	51.36
169.38	168.64	168.23		56.58	56.55	52.96
169.70	169.35	168.51		57.52	57.56	53.60
169.86	169.72	168.99		61.36	61.68	56.90
170.02	169.77	169.46		63.20	63.00	58.37
170.74	170.02	169.68		63.83	63.76	62.99
170.81	170.46	169.80		64.43	64.48	63.54
171.97	170.63	170.33		65.61	65.68	64.12
173.15	172.74	170.53		66.38	66.41	65.08
174.48	173.77	172.55		66.74	66.77	65.64
175.37	174.19	173.40		67.72	67.63	66.72
175.86	175.23	173.64		68.14	68.31	67.36
176.95	176.63	175.10		68.62	68.71	67.54

178.10	177.89	176.26	70.29	70.40	68.55
178.74	178.15	177.78	71.22	71.08	68.72
179.00	178.82	178.00	72.26	72.39	70.37
180.09	179.96	178.85	73.17	73.01	71.16
180.85	180.49	179.52	73.52	73.44	72.19
181.57	181.57	180.15	73.88	73.87	72.97
181.97	182.00	181.33	77.42	77.54	73.37
182.96	182.17	181.90	79.48	79.52	73.83
183.19	183.35	182.08	79.90	79.79	75.14
184.16	183.88	183.00	80.83	80.61	78.90
185.61	185.32	183.74	81.94	82.14	79.73
185.91	185.81	185.21	82.65	82.55	80.87
186.15	186.51	185.77	83.02	83.05	81.24
187.08	187.01	186.18	83.88	83.99	82.53
187.52	187.39	186.66	84.68	84.62	82.96
187.74	187.79	187.18	87.82	87.76	83.01
188.24	188.22	187.44	88.00	88.42	84.58
188.59	188.56	188.11	89.02	89.56	84.62
189.27	189.34	188.36	91.00	91.17	87.57
189.77	189.58	188.93	91.27	91.47	89.40
190.54	190.33	189.38	91.45	91.57	90.28
190.83	190.72	190.09	91.93	92.07	90.95
191.99	192.04	190.38	92.51	92.69	91.27
192.27	192.24	191.84	93.90	93.54	91.56
193.00	192.46	191.95	94.30	94.20	92.10
193.39	193.19	192.23	94.61	94.75	92.44
193.71	193.64	193.01	94.82	94.96	93.64
193.88	193.67	193.37	95.63	95.67	94.46
194.61	194.01	193.43	95.80	95.91	94.72
195.27	194.36	193.70	96.15	96.44	94.95
197.81	197.83	194.33	96.70	96.70	95.78
197.97	198.01	197.69	97.06	97.20	95.83
198.41	198.41	197.79	97.19	97.24	96.65
198.99	198.79	198.15	97.65	97.50	96.84
199.75	199.61	198.50	97.94	97.79	97.18
200.26	200.12	199.59	98.00	98.23	97.33
200.59	200.25	199.85	98.52	98.47	97.58
201.67	201.59	199.96	98.98	99.07	98.28
202.11	201.98	201.22	99.29	99.37	98.33
203.18	202.91	201.70	99.39	99.55	98.59
203.32	203.19	202.83	100.38	100.37	98.80
204.00	203.83	203.02	100.42	100.45	99.25
204.23	204.05	203.73	100.89	100.95	99.80
205.59	205.35	203.94	102.24	102.45	100.15

205.96	205.83	205.26	103.92	104.25	100.58
206.14	206.07	205.40	105.09	105.12	101.49
206.70	206.34	205.75	105.43	105.78	102.23
207.31	207.09	206.32	105.71	105.88	104.23
207.44	207.40	206.82	105.97	105.98	104.85
208.90	209.11	207.18	106.32	106.56	105.07
209.22	209.12	208.50	106.70	106.70	105.98
209.97	209.53	208.53	107.14	107.34	106.16
213.04	212.87	209.03	107.55	107.59	106.80
213.47	213.38	212.65	107.74	108.37	107.37
214.69	214.76	213.35	108.92	109.28	107.51
215.22	215.32	214.41	109.44	109.68	107.69
215.89	215.89	214.75	109.95	109.76	108.38
216.15	216.09	215.16	110.57	110.83	109.27
216.58	216.20	215.47	111.08	111.17	109.84
218.33	216.82	215.82	111.46	111.59	110.09
218.95	217.63	216.45	111.64	111.74	111.14
219.87	219.55	217.07	112.16	112.32	111.38
220.30	219.97	219.54	112.81	113.23	111.47
222.40	222.47	219.84	113.47	113.51	111.73
223.69	223.94	222.23	113.89	113.76	112.09
224.77	224.82	223.64	114.36	114.66	113.34
225.06	225.36	224.51	115.18	115.13	113.68
225.49	225.64	224.83	115.46	115.44	113.87
227.31	227.40	225.15	115.74	115.80	114.75
227.69	227.74	227.01	115.93	115.93	115.26
229.58	229.49	227.32	116.08	116.16	115.39
229.90	229.72	229.29	116.42	116.86	115.72
230.65	230.60	229.65	116.79	116.95	115.80
230.92	231.03	230.43	117.31	117.16	115.96
232.29	232.33	230.81	117.92	117.65	116.84
232.71	232.90	231.76	118.35	118.19	117.05
233.24	233.41	232.00	118.69	118.63	117.40
234.17	234.43	233.06	119.00	119.10	118.33
234.52	234.45	233.95	119.30	119.22	118.42
238.34	238.27	234.28	119.42	119.50	118.69
239.11	239.32	237.90	119.63	119.61	118.89
239.79	239.68	238.75	119.65	119.87	119.30
240.90	240.96	239.46	120.00	119.99	119.43
241.91	241.64	240.48	120.32	120.30	119.60
242.53	242.60	241.45	120.58	120.52	119.74
243.86	243.78	242.10	120.84	121.07	119.87
244.71	244.46	243.48	121.02	121.54	120.33
246.43	246.64	244.31	122.98	122.78	120.51

247.01	246.86	245.89	123.37	123.43	121.09
247.93	247.77	246.57	123.90	124.07	123.07
248.41	247.94	247.31	124.26	124.60	123.46
248.99	248.79	247.63	124.77	124.87	123.89
249.08	248.80	248.53	125.30	125.51	123.93
249.12	248.97	248.61	125.67	125.96	124.81
249.26	249.14	248.65	126.20	126.16	125.29
249.75	249.46	248.91	126.98	126.69	125.91
249.96	249.66	249.38	127.50	127.45	125.96
250.94	250.57	249.52	127.63	127.99	126.62
250.98	250.71	250.23	128.27	129.05	127.23
251.66	251.42	250.34	129.93	129.52	127.91
251.96	251.69	251.04	130.10	130.02	128.17
252.46	252.20	251.39	130.29	130.24	129.75
253.03	252.98	252.19	130.83	130.81	129.94
253.36	253.26	252.40	131.15	131.14	130.37
253.49	253.58	252.86	131.27	131.25	130.62
254.02	253.65	253.00	131.58	131.58	130.85
254.72	254.49	253.39	131.89	131.96	131.09
254.96	254.61	254.21	131.93	132.03	131.54
255.87	255.75	254.40	132.46	132.66	131.68
256.08	255.84	255.12	133.16	133.22	131.90
256.25	255.99	255.73	133.42	133.43	132.96
256.41	256.37	255.84	133.76	133.83	133.07
257.07	256.64	256.06	133.87	133.84	133.32
257.76	257.40	256.35	134.08	134.07	133.54
258.27	257.96	257.24	134.29	134.37	133.80
259.58	259.16	257.57	135.04	134.47	134.04
261.06	260.73	258.82	135.17	135.53	134.41
264.28	264.17	260.37	135.90	136.07	134.73
265.56	265.92	264.06	136.28	136.45	135.63
518.15	346.87	265.03	136.96	136.92	135.87
632.74	430.40	347.73	137.13	137.06	136.22
867.01	524.22	526.01	137.36	137.55	136.74
3613.89	3588.45	3508.17	137.79	137.72	137.04
			137.98	137.89	137.26
			138.58	138.05	137.55
			138.84	138.71	137.77
			139.27	139.14	138.00
			139.46	139.34	138.43
			139.75	139.79	138.92
			140.32	140.07	139.11
			140.72	140.65	139.33
			140.92	141.12	140.46

141.40	141.15	140.61
142.19	141.79	140.82
142.83	142.63	140.95
143.35	143.22	142.28
143.38	143.28	143.12
143.60	143.74	143.21
143.94	143.97	143.26
144.03	144.05	143.54
144.28	144.23	143.81
144.60	144.57	143.92
145.05	145.14	144.31
145.69	145.47	144.90
146.05	146.02	144.98
146.40	146.24	145.98
146.49	146.44	146.15
146.76	146.49	146.29
147.07	147.02	146.42
147.95	148.03	146.81
148.38	148.56	147.91
148.80	148.68	148.20
149.43	149.14	148.57
149.84	149.69	148.91
150.15	150.10	149.36
150.82	150.82	149.49
151.13	151.15	150.00
151.63	151.53	150.25
152.19	151.74	150.88
152.54	152.43	151.26
153.13	152.73	152.18
153.76	153.76	152.39
154.01	153.97	153.42
154.38	154.37	153.65
154.59	154.52	153.98
155.15	155.43	154.07
155.53	155.66	155.19
155.85	155.91	155.50
156.40	156.29	155.52
156.68	156.57	155.87
156.93	156.68	156.09
157.13	156.99	156.72
157.55	157.24	156.86
157.64	157.70	157.27
158.08	158.00	157.37
158.50	158.33	157.88

158.62	158.77	158.03
159.44	159.31	158.43
159.87	159.62	158.89
160.03	159.83	159.09
160.34	160.01	159.46
160.85	160.58	160.10
160.91	160.75	160.52
161.30	160.96	160.63
161.92	161.54	160.86
162.20	162.08	160.92
163.69	163.41	161.87
164.08	163.70	163.47
164.67	164.41	163.85
165.17	164.75	164.09
166.22	166.04	164.82
166.66	166.51	166.05
168.45	167.33	166.53
168.64	168.58	167.98
169.89	168.72	168.49
170.79	169.94	169.57
171.28	171.24	170.37
172.19	171.99	170.74
172.53	172.38	171.57
173.02	172.78	172.32
173.10	172.98	172.57
174.10	173.83	172.78
174.71	174.50	173.63
174.80	174.64	174.31
175.31	175.07	174.64
175.71	175.40	175.03
176.52	175.75	175.42
178.65	178.51	176.24
178.94	178.63	178.23
179.31	179.00	178.46
179.40	179.29	178.85
179.73	179.46	178.95
179.94	179.83	179.44
181.24	181.27	179.89
181.45	181.43	180.95
182.45	182.23	181.07
182.73	182.71	182.03
184.50	183.99	182.33
185.49	185.19	183.92
185.99	185.51	184.83

186.16	186.15	185.61
187.50	186.81	185.87
187.66	187.59	187.19
188.64	187.94	187.31
188.94	188.73	188.34
189.15	188.92	188.58
189.60	189.12	188.82
190.34	190.44	189.36
190.96	190.65	190.06
192.13	191.98	190.67
192.48	192.19	191.54
192.94	192.87	192.10
194.79	194.78	192.34
196.70	195.62	194.65
198.34	197.49	196.11
198.63	198.59	197.98
199.64	198.75	198.07
199.85	199.56	199.21
200.54	200.55	199.60
203.10	201.30	200.13
203.18	203.11	202.58
203.63	203.14	202.74
203.97	203.49	203.31
204.23	204.04	203.78
204.61	204.34	203.94
206.50	204.74	204.37
207.54	206.46	205.95
208.16	207.47	207.21
209.04	208.16	207.76
209.28	209.10	208.75
210.04	209.30	208.87
211.24	210.20	209.82
211.51	211.24	210.58
212.10	211.82	211.09
212.34	212.16	211.29
213.57	212.64	211.78
213.98	213.59	212.86
214.37	213.68	213.22
214.67	214.37	213.89
215.05	214.79	214.17
216.52	215.13	214.39
216.96	216.51	216.10
217.84	217.08	216.60
218.26	217.76	217.43

218.57	218.40	217.75
220.04	218.47	218.06
220.69	220.60	219.22
221.22	220.79	220.15
222.29	221.22	220.44
222.30	222.25	222.16
224.49	222.41	222.23
225.50	224.62	223.52
226.16	225.01	224.05
227.39	226.30	225.72
228.38	227.96	226.83
228.54	228.31	227.80
229.08	228.67	228.17
231.76	229.30	228.83
233.11	231.65	231.25
234.90	233.19	232.90
235.95	234.91	234.01
237.86	235.63	234.97
239.22	237.93	237.51
241.96	239.13	238.43
242.00	241.68	241.22
243.09	241.88	241.51
243.33	242.95	242.36
244.87	243.21	242.63
244.90	244.85	243.99
245.38	244.97	244.49
245.61	245.24	244.61
245.94	245.44	244.87
246.12	245.72	245.29
246.29	245.86	245.46
246.63	245.95	245.67
246.91	246.49	245.83
247.12	246.78	246.35
247.19	246.95	246.52
247.26	247.08	246.72
247.86	247.16	246.82
248.24	247.79	247.30
248.43	248.26	247.57
248.95	248.49	247.83
249.47	248.81	248.36
250.89	249.09	248.52
250.93	250.90	250.28
251.34	251.01	250.58
252.41	251.07	250.66

254.72	252.05	251.29
255.08	254.29	253.31
257.67	255.13	254.39
259.64	257.17	257.01
263.73	259.74	259.21
456.56	263.83	262.62
556.74	399.95	359.12
938.45	483.24	547.76
3627.22	3576.43	3517.11

Table S11. Gibbs free energy change of NORR on Cd/Cu(553) with solvation effect and dipole correction.

Method	*NO	*HNO	*HNOH	*H ₂ NOH	*NH ₂	*NH ₃	NH ₃ desorption
DFT	-0.43	0.00	-0.91	-0.31	-0.96	-1.58	0.15
DFT+solvation effect	-0.38	-0.15	-0.98	-0.50	-0.79	-1.50	0.16
DFT+dipole correction	-0.30	-0.01	-0.91	-0.31	-1.11	-1.45	0.11

Table S12. Optimal hyper-parameters of five different models.

Model	hyper-parameters
KRR	alpha=0.0013902870612802368, degree=2, gamma=0.36000000000000004, kernel='rbf'
LASSO	alpha=0.00010032248675910343, max_iter=350 C=7.471598965125458,
SVR	degree=4, epsilon=0.16000000000000003
RFR	max_depth=15, n_estimators=40 base_score=None, booster=None, callbacks=None, colsample_bylevel=None, colsample_bynode=None, colsample_bytree=0.8, device=None, early_stopping_rounds=None, enable_categorical=False, eval_metric=None, feature_types=None, gamma=0, grow_policy=None, importance_type=None, interaction_constraints=None, learning_rate=0.3, max_bin=None, max_cat_threshold=None, max_cat_to_onehot=None, max_delta_step=None, max_depth=10, max_leaves=None, min_child_weight=5, missing=nan, monotone_constraints=None, multi_strategy=None, n_estimators=80, n_jobs=32, num_parallel_tree=None, random_state=None
XGBoost	

Table S13. Parameters of MBTR.

Function	Parameters
species	["H", "O", "N", "Sc", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Y", "Zr", "Nb", "Mo", "Tc", "Ru", "Rh", "Pd", "Ag", "Cd", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg"]
periodic geometry	True
grid	{"function": "cosine"}
weighting	{'min': -1.0, 'max': 1.0, 'sigma': 0.1, 'n': 10}
normalization	{'function': 'exp', 'r_cut': 10, 'threshold': 1e-3}
sparse	'valle_ogonov'
	False

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