

Supporting Information for

**Examination of the Brønsted–Evans–Polanyi Relationship for the Hydrogen
Evolution Reaction on Transition Metals Based on Constant Electrode
Potential Density Functional Theory**

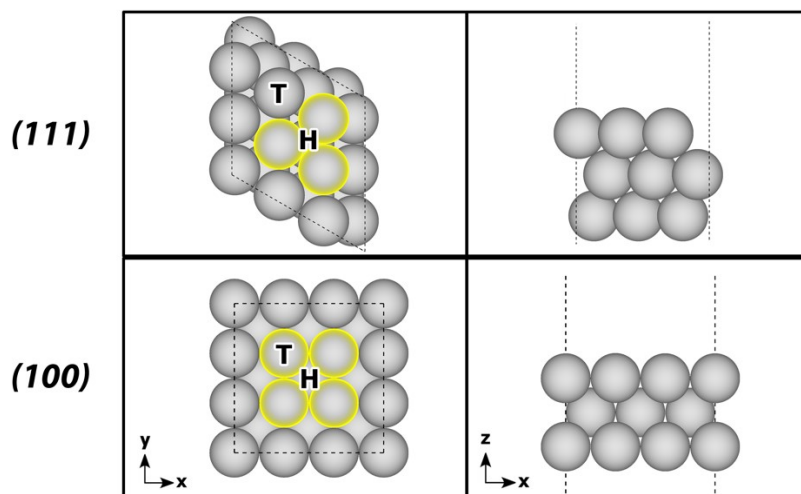
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Computational Details

The PBE functional¹ with projector augmented wave pseudopotentials (400 eV energy cutoff)^{2, 3} as implemented in the Vienna ab initio Simulation Package⁴⁻⁷ was used to perform all calculations. A Gaussian-smearing method with a parameter of $k_B T = 0.1$ eV was used to accelerate SCF convergence, and the calculated electronic energies were extrapolated to $k_B T = 0$ eV. A Monkhorst-Pack k -point net of $3 \times 3 \times 1$ was chosen to sample the reciprocal space for the slab calculations. Using a denser $5 \times 5 \times 1$ k -point net leads to less than 0.02 eV variation in the hydrogen binding energy on the top site. This indicates that k -point net of $3 \times 3 \times 1$ is enough to obtain accurate energetics. The (111) and (100) index surfaces of the eight metals were simulated using a 3×3 three-layer slab (Figure S1). During the geometric optimizations, the top two layers and adsorbates were allowed to relax, whereas the bottom layer was fixed in its bulk position. The bulk cell parameter for Ag, Au, Cu, Ni, Pd, Rh, Ir, and Pt are 4.086, 4.073, 3.615, 3.516, 3.890, 3.804, 3.900, and 3.944 Å, respectively. A vacuum of at least 30 Å was introduced to avoid interactions between replicas along the z -direction. Spin-polarized wavefunction was used for Ni and Pd, whereas spin-unpolarized one was used for the other metals.

Figure S1. Top and side views of (111) and (100) index surface of the slab model. The top (T) and hollow (H) sites are marked.



To simulate the electrochemical systems, the approach proposed by Head-Gordon et al.⁸ was applied in this study. In this model, the Fermi energy is adjusted to a target value by changing the number of electrons in the system during each step of the geometry optimization. This allows one to fix the work function and hence the electrode potential in the calculations. The U of the electrode was calculated by relating the work function (Φ) of the system to the experimental work function of the standard hydrogen electrode (SHE) as follows:

$$U = \frac{\Phi - \Phi_{\text{SHE}}}{e}.$$

A value of 4.3 eV, suggested by Anderson and co-workers in their theoretical study, was used for Φ_{SHE} .⁹ To provide a more realistic description of the electrochemical double layer and to maintain charge neutrality of the cell, the linear Poisson-Boltzmann implicit solvation model with a Debye screening length of 3.0 Å (corresponding to 1.0 M concentration of the electrolyte) as implemented in VASPsol was used.¹⁰ All the energetics reported in this study were calculated under the condition of $U = -0.5 \text{ V}_{\text{SHE}}$ and $\text{pH} = 0$.

A proton solvated by the water cluster ($\text{H}^+\cdot 4\text{H}_2\text{O}$, the Eigen proton solvated model) was transferred to * and *H to locate the transition states (TSs) of the Volmer and Heyrovsky steps. This approach has been used by a previous theoretical study and the calculated barriers were in good agreement with that by transferring a proton from water bilayers to the surface.¹¹ The kinetic barriers were obtained by referencing the free energy of the transition state to the free energy of the initial state solvated by four explicit water molecules plus the free energy of a proton-electron pair.¹² The charge transfer coefficient is assumed to be 0.5 for the transition states, which is in the range of the experimentally determined value of 0.3 to 0.7.¹³

The free energies of the slab systems were calculated based on the equation as follows:

$$G = E_{elect} + ZPVE + \sum_v \frac{hv}{e^{hv/k_b T} - 1} - T \times S_{vib}$$

The vibrational frequencies were only evaluated for surface adsorbates by evaluating the partial Hessian matrix via the finite difference approach to obtain the zero-point vibrational energy (ZPVE). The low vibrational modes with a frequency $< 50 \text{ cm}^{-1}$ were adjusted to have a value of 50 cm^{-1} to avoid a spurious contribution to the entropy. The constant electrode potential method applied in this work leads to different numbers of electrons for each stationary point along the reaction path, and therefore the calculated G needs to be corrected based on the following equation:

$$G^{corr}(U) = G(U) - (N_{e,U} - N_{e,0})\mu_e(U),$$

where $N_{e,U}$ and $N_{e,0}$ are the number of electrons in the system under the target U and zero charge, respectively, and $\mu_e(U)$ is the chemical potential of the electrons under U and is equal to the Fermi energy.

The vibrational frequencies for each stationary point were examined. Each transition state has one imaginary frequency, corresponding to the reaction direction. In addition, there are no imaginary frequencies for reactants, intermediates, and products. The transition states were located using the dimer method^{14,15} and further verified by vibrational frequency calculations where only one imaginary frequency was present.

The ALMO-EDA analysis was performed using the Q-Chem package with the same PBE functional. For the basis sets, LanL2DZ was used for Pt, and 6-31G** was used for the others. During optimization, the coordinates for all Pt atoms were fixed in their bulk positions.

References

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2. Calculated Free Energies and its Energy Components

Table S1. Calculated free energies for each species in the aqueous phase under $-0.5 V_{\text{SHE}}$

Metal(111)	E_{SCF}	Added e^-	$E_{\text{SCF}}^{\text{corr}}$	ZPE	H_{vib}	S_{vib}	G(eV)
Pt(111)_Rf_sur	-220.93633	1.52521	-213.65940	14.64274	1.92829	14.64493	-213.13067
Pt(111)_Rf_top	-224.55863	1.48910	-217.45369	18.46403	2.56545	17.80442	-216.76816
Pt(111)_Rf_fcc	-225.50270	1.63691	-217.69202	18.01093	2.08621	14.38132	-217.00436
Pt(111)_Volmer	-223.19546	1.21124	-217.41700	18.44291	1.20571	7.32290	-216.65959
Pt(111)_Heyrovsky	-225.50296	1.15904	-219.97202	22.42351	1.97957	12.72157	-219.07821
Ir(111)_Rf_sur	-286.26433	1.17514	-280.75375	14.61415	1.92114	14.57220	-280.22128
Ir(111)_Rf_top	-290.22813	1.20459	-284.57969	18.71933	2.23352	14.77659	-283.86236
Ir(111)_Rf_fcc	-290.69583	1.30407	-284.58105	18.10429	2.05950	14.28400	-283.89021
Ir(111)_Volmer	-288.25104	0.86556	-284.19200	17.43533	1.40373	8.68950	-283.48736
Ir(111)_Heyrovsky	-291.29638	0.85506	-287.28897	22.54165	2.41785	17.17429	-286.42857
Rh(111)_Rf_sur	-245.31237	0.91948	-241.00176	14.56938	1.94229	14.73520	-240.47441
Rh(111)_Rf_top	-248.96949	0.94712	-244.52825	17.94756	2.57840	18.11777	-243.87405
Rh(111)_Rf_fcc	-249.55627	1.00203	-244.85915	18.57971	1.96594	13.55447	-244.14422
Rh(111)_Volmer	-247.36344	0.67734	-244.18800	17.46260	1.40206	8.47334	-243.47946

Rh(111)_Heyrovsky	-250.20092	0.57845	-247.48932	22.62012	2.32622	17.28532	-246.63093
Pd(111)_Rf_sur	-195.43111	1.11057	-190.29284	14.59523	1.94233	14.74496	-189.76341
Pd(111)_Rf_top	-199.05281	1.15026	-193.73033	17.65697	2.88042	22.47315	-193.12983
Pd(111)_Rf_fcc	-200.08399	1.23244	-194.38124	18.51935	2.00591	14.34487	-193.67532
Pd(111)_Volmer	-198.12761	0.95950	-193.68695	18.41667	1.62941	10.79804	-192.95722
Pd(111)_Heyrovsky	-200.02113	0.72070	-196.68955	22.02023	2.30898	17.76632	-195.86413
Ni(111)_Rf_sur	-198.99468	0.71322	-195.70274	14.64180	1.92071	14.56476	-195.17000
Ni(111)_Rf_top	-202.58162	0.75778	-199.08462	17.60302	2.78755	21.99448	-198.48001
Ni(111)_Rf_fcc	-203.07080	0.75777	-199.57384	18.82525	1.94304	13.81852	-198.84798
Ni(111)_Volmer	-201.42651	0.54907	-198.89272	17.43509	1.33582	7.68758	-198.17809
Ni(111)_Heyrovsky	-203.80245	0.37082	-202.09100	22.45749	2.31390	17.94830	-201.24876
Cu(111)_Rf_sur	-154.56520	0.61283	-151.76867	14.61966	1.92180	14.57429	-151.24104
Cu(111)_Rf_top	-157.49892	0.57964	-154.85414	17.36267	2.75702	21.80432	-154.25930
Cu(111)_Rf_fcc	-158.44158	0.66139	-155.42353	18.82993	1.89928	13.22214	-154.69197
Cu(111)_Volmer	-156.58401	0.44596	-154.54860	17.06743	1.80842	12.31407	-153.88921
Cu(111)_Heyrovsky	-158.94434	0.20017	-158.03068	22.63633	2.25177	17.07468	-157.17209
Au(111)_Rf_sur	-145.67248	1.10547	-140.75590	14.62195	1.93085	14.65900	-140.23164
Au(111)_Rf_top	-148.75603	1.12775	-143.73991	17.62769	2.73124	20.07050	-143.11652
Au(111)_Rf_fcc	-149.61355	1.25089	-144.05022	17.90594	2.21927	16.35986	-143.38871
Au(111)_Volmer	-148.17064	1.00203	-143.71431	18.60363	1.62301	10.68050	-142.97523
Au(111)_Heyrovsky	-149.67592	0.64456	-146.83973	21.49745	1.97000	12.75602	-145.98693
Ag(111)_Rf_sur	-128.31132	0.52951	-126.06201	14.55317	1.97129	14.99443	-125.53721
Ag(111)_Rf_top	-131.27483	0.56692	-128.86735	17.27431	2.68419	21.08282	-128.27697
Ag(111)_Rf_fcc	-132.25486	0.69135	-129.31883	18.26713	1.94008	13.36193	-128.61641
Ag(111)_Volmer	-130.38624	0.43859	-128.52311	17.27082	1.96389	13.67562	-127.86575
Ag(111)_Heyrovsky	-132.42951	0.04512	-132.23781	21.25694	2.24018	15.97638	-131.42534

Metal(100)	E_{SCF}	Added e⁻	E_{SCF}^{corr}	ZPE	H_{vib}	S_{vib}	G(eV)
Pt(100)_Rf_sur	-217.51274	1.73784	-208.91217	14.70357	1.89690	14.40706	-208.37632
Pt(100)_Rf_top	-221.56139	1.78357	-212.73183	17.99986	2.85807	22.24210	-212.11295
Pt(100)_Rf_fcc	-222.22012	1.85326	-213.04852	18.63080	2.06783	14.02902	-212.33372
Pt(100)_Volmer	-219.30464	1.35230	-212.61089	17.64487	1.32542	8.63552	-211.89986
Pt(100)_Heyrovsky	-222.30987	1.40320	-215.36361	22.28850	2.38628	18.00098	-214.52624
Ir(100)_Rf_sur	-281.51643	1.58713	-273.81742	14.62731	1.92668	14.59757	-273.29080
Ir(100)_Rf_top	-285.50161	1.59873	-277.74409	18.31064	2.49397	16.84211	-277.05548
Ir(100)_Rf_fcc	-285.89899	1.64641	-277.91242	18.72112	2.03955	13.59817	-277.18547
Ir(100)_Volmer	-283.08802	1.18536	-277.33725	17.84276	1.37757	9.14741	-276.62199
Ir(100)_Heyrovsky	-286.28640	1.20530	-280.43768	22.37672	2.42081	18.86569	-279.60616

Rh(100)_Rf_sur	-241.70964	1.19829	-235.89602	14.56438	1.93703	14.70480	-235.37446
Rh(100)_Rf_top	-245.50598	1.23232	-239.52528	17.78243	2.72032	21.20005	-238.91488
Rh(100)_Rf_fcc	-245.46286	1.18437	-239.71535	16.74964	2.30374	15.33468	-239.09194
Rh(100)_Volmer	-242.55746	0.70076	-239.15737	17.21379	1.46063	9.37314	-238.46871
Rh(100)_Heyrovsky	-246.16825	0.75936	-242.48361	22.53461	2.27487	17.13259	-241.62918
Pd(100)_Rf_sur	-192.31828	1.14334	-186.85563	14.56166	1.92941	14.64417	-186.33413
Pd(100)_Rf_top	-196.13525	1.21182	-190.34408	17.67476	2.80449	21.97339	-189.73590
Pd(100)_Rf_fcc	-197.18035	1.32397	-190.85270	16.45675	2.36451	15.60072	-190.23544
Pd(100)_Volmer	-194.71200	0.92936	-190.27087	18.28590	1.34048	8.23995	-189.52628
Pd(100)_Heyrovsky	-196.85163	0.71805	-193.41160	21.78917	2.27470	17.04614	-192.58838
Ni(100)_Rf_sur	-195.75115	0.83042	-191.79138	14.86659	1.73111	11.91838	-191.22428
Ni(100)_Rf_top	-199.30264	0.85003	-195.24910	17.73502	2.63557	20.21348	-194.62787
Ni(100)_Rf_fcc	-200.36638	0.96256	-195.77593	17.66693	1.87666	11.97748	-195.08730
Ni(100)_Volmer	-197.24135	0.49913	-194.86115	17.12594	1.40394	8.31232	-194.16504
Ni(100)_Heyrovsky	-200.07911	0.39305	-198.20473	22.41270	2.18238	16.53542	-197.35188
Cu(100)_Rf_sur	-151.99743	0.54926	-149.41393	14.67832	1.86295	13.25707	-148.86403
Cu(100)_Rf_top	-155.02805	0.53980	-152.48932	17.45942	2.67115	20.67219	-151.88420
Cu(100)_Rf_fcc	-156.29465	0.69532	-153.02428	17.47676	1.97152	12.78981	-152.34193
Cu(100)_Volmer	-152.96701	0.18344	-152.10403	16.76096	1.65115	10.85708	-151.44592
Cu(100)_Heyrovsky	-155.60896	-0.02003	-155.70317	21.01345	2.28255	17.27534	-154.91621
Au(100)_Rf_sur	-144.57341	1.34479	-138.43404	14.35620	2.16068	17.78882	-137.94364
Au(100)_Rf_top	-148.36108	1.50585	-141.48567	17.58779	2.78609	21.86816	-140.88911
Au(100)_Rf_fcc	-148.55906	1.47449	-141.82595	18.36622	2.16307	14.88967	-141.13219
Au(100)_Volmer	-146.72220	1.16038	-141.42518	18.39340	1.45169	9.69617	-140.68993
Au(100)_Heyrovsky	-148.56497	0.84323	-144.71428	21.19300	1.93946	11.91813	-143.86518
Ag(100)_Rf_sur	-126.53907	0.49595	-124.39240	14.37332	2.14614	17.35339	-123.89791
Ag(100)_Rf_top	-128.81217	0.37542	-127.18698	17.23471	2.67225	21.03457	-126.59858
Ag(100)_Rf_fcc	-129.91402	0.55945	-127.49171	16.59584	2.35632	15.87463	-126.87331
Ag(100)_Volmer	-127.33112	0.10807	-126.86328	17.03765	1.62137	10.66839	-126.19203
Ag(100)_Heyrovsky	-129.60705	-0.23842	-130.63965	20.68263	2.17484	15.76642	-129.85221

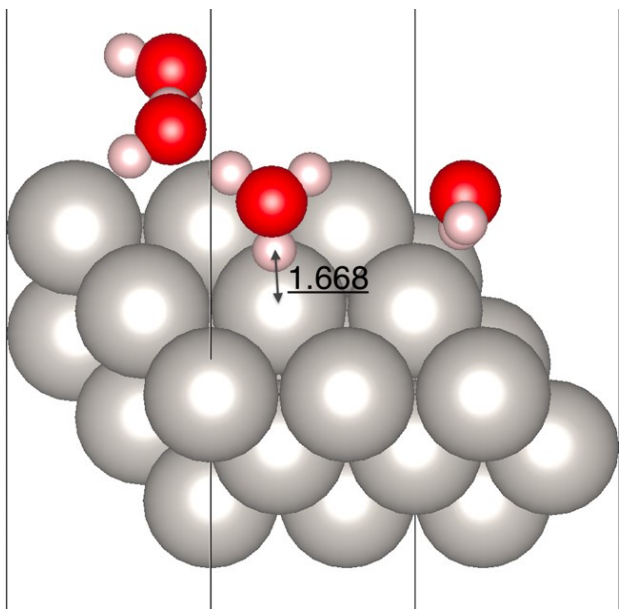
Single-Atom Alloy(111)	E_{SCF}	Added e ⁻	$E_{\text{SCF}}^{\text{corr}}$	ZPE	H_{vib}	S_{vib}	G(eV)
Pt@Au_Rf_sur	-148.77562	1.12866	-143.37114	14.64352	1.89336	14.38704	-142.83996
Pt@Au_Rf_top	-152.24223	1.09500	-146.99959	18.35919	2.48627	16.78539	-146.31256
Pt@Au_Rf_fcc	-152.84434	1.24353	-146.88895	17.91297	2.28007	15.80212	-146.21751
Pt@Au_Volmer	-150.81419	0.84285	-146.77881	17.96104	1.27558	8.02186	-146.04830
Pt@Au_Heyrovsky	-153.26506	0.72474	-149.79500	22.22447	2.01522	13.27562	-148.91544
Rh@Au_Rf_sur	-149.90476	1.19384	-144.19701	14.54975	1.94425	14.76873	-143.67262

Rh@Au_Rf_top	-153.13619	1.12318	-147.76683	18.21179	2.44130	16.49190	-147.08435
Rh@Au_Rf_fcc	-153.53580	1.22150	-147.69654	17.86869	2.22003	15.04124	-147.01979
Rh@Au_Volmer	-151.20342	0.78924	-147.43046	17.40698	1.40341	8.76848	-146.72808
Rh@Au_Heyrovsky	-154.24541	0.72362	-150.78622	21.97497	2.29103	17.09558	-149.95487
Pd@Au_Rf_sur	-148.13505	1.10487	-142.85410	14.60597	1.93125	14.65271	-142.32634
Pd@Au_Rf_top	-151.39479	1.13006	-145.99423	17.58422	2.76514	21.61598	-145.39114
Pd@Au_Rf_fcc	-152.10534	1.21431	-146.30252	18.14706	2.02392	14.13505	-145.61049
Pd@Au_Volmer	-150.52030	0.98134	-145.82909	18.46274	1.61215	9.97015	-145.08742
Pd@Au_Heyrovsky	-151.84389	0.55160	-149.20768	21.56258	1.92182	11.44693	-148.33724
Ni@Au_Rf_sur	-148.05020	1.17608	-142.43936	14.66030	1.92440	14.61173	-141.90901
Ni@Au_Rf_top	-151.12757	1.14340	-145.67332	17.64317	2.75115	21.63839	-145.06857
Ni@Au_Rf_fcc	-151.78516	1.22423	-145.94485	18.08230	2.05168	14.19914	-145.25526
Ni@Au_Volmer	-149.56301	0.88523	-145.33905	17.62797	1.54403	10.04584	-144.63750
Ni@Au_Heyrovsky	-152.55397	0.77104	-148.87434	22.09545	2.27790	16.96420	-148.03664
Cu@Au_Rf_sur	-146.57523	1.14455	-141.11618	14.66867	1.92685	14.63374	-140.58565
Cu@Au_Rf_top	-149.62277	1.18751	-143.95633	17.43489	2.70656	21.28722	-143.35801
Cu@Au_Rf_fcc	-150.21620	1.19522	-144.51345	18.12668	2.00754	14.40191	-143.82646
Cu@Au_Volmer	-148.29993	0.97739	-143.63612	17.18442	1.92825	13.63016	-142.98346
Cu@Au_Heyrovsky	-151.00279	0.75037	-147.42217	22.14126	1.96061	12.83428	-146.54288

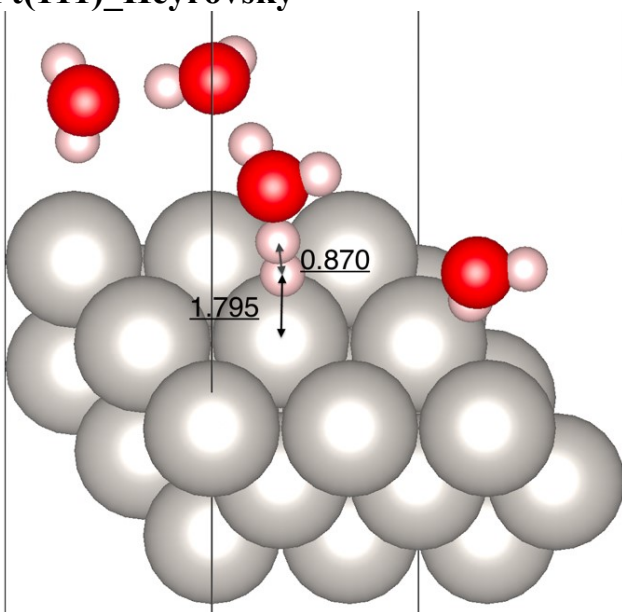
3. Transition State Structures

Metal(111)

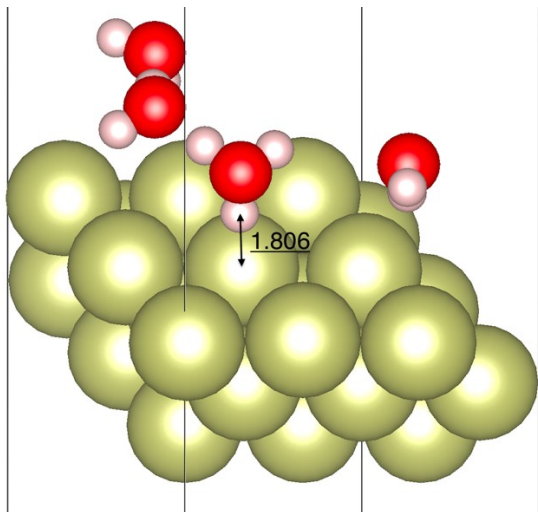
Pt(111)_Volmer



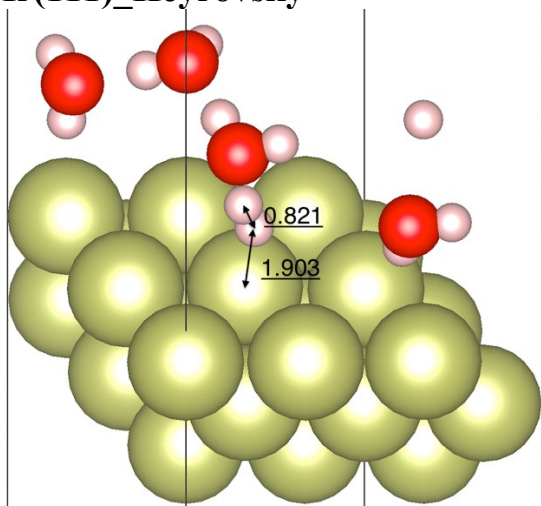
Pt(111)_Heyrovsky



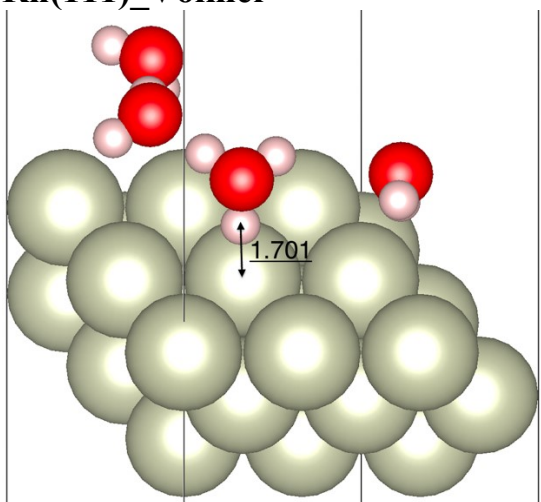
Ir(111)_Volmer



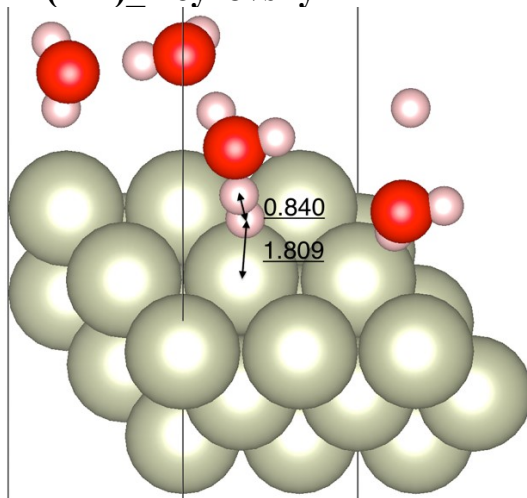
Ir(111)_Heyrovsky



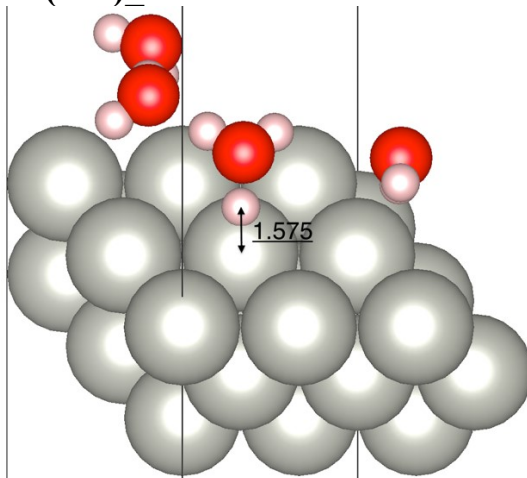
Rh(111)_Volmer



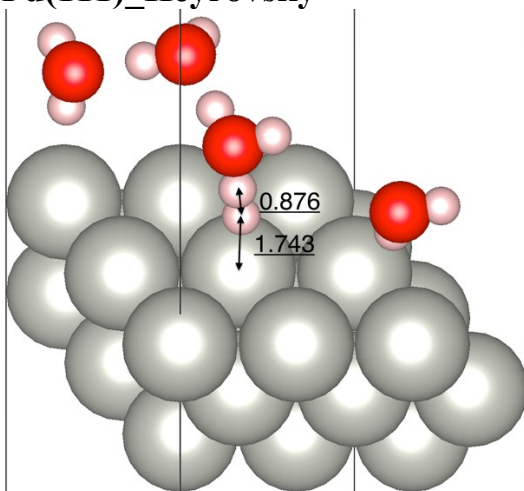
Rh(111)_Heyrovsky



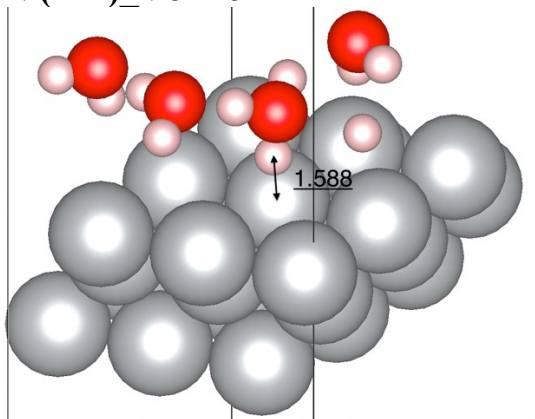
Pd(111)_Volmer



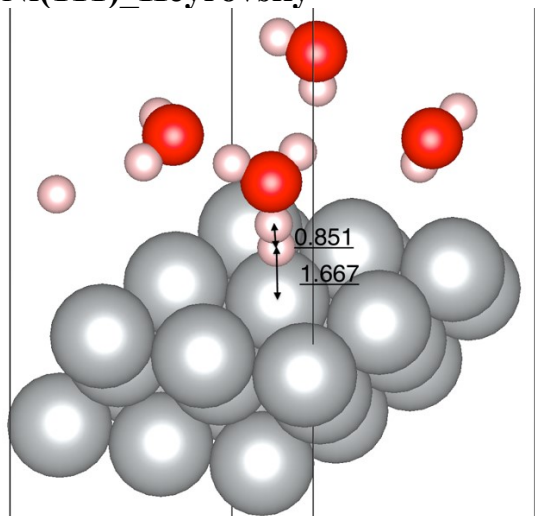
Pd(111)_Heyrovsky



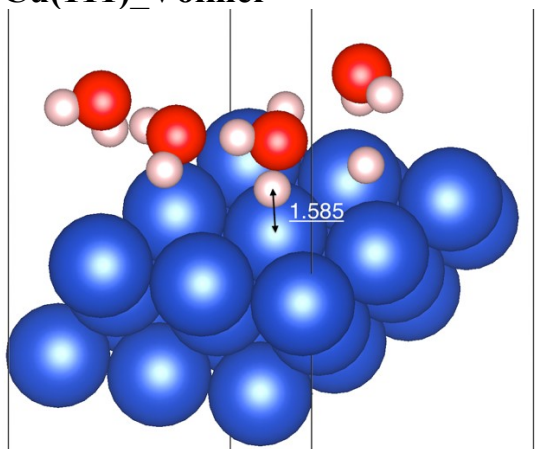
Ni(111)_Volmer



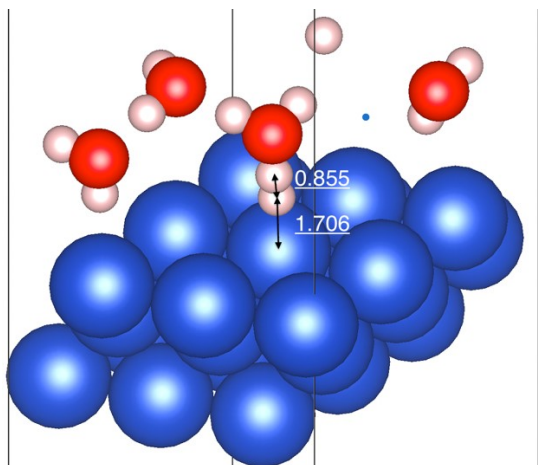
Ni(111)_Heyrovsky



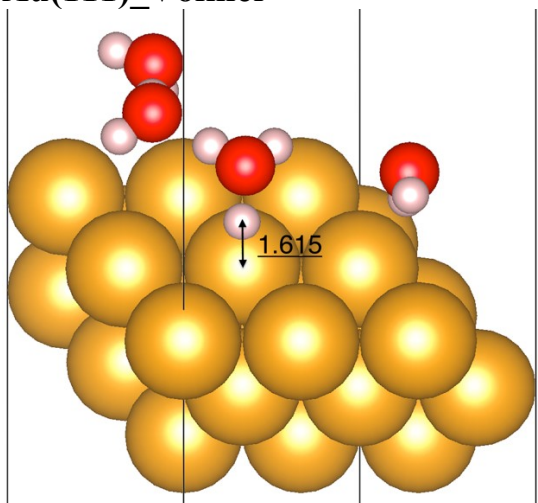
Cu(111)_Volmer



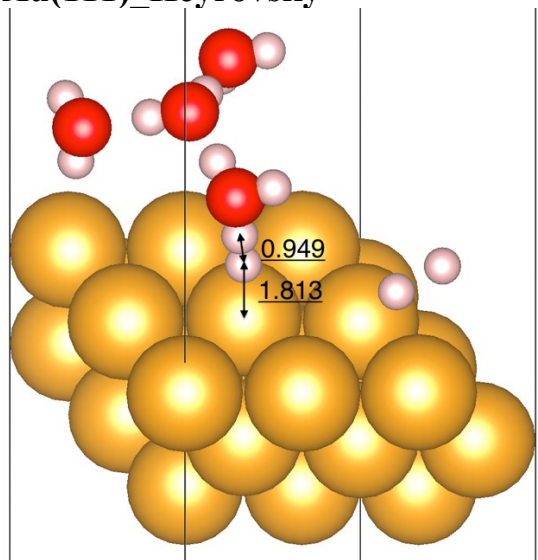
Cu(111)_Heyrovsky



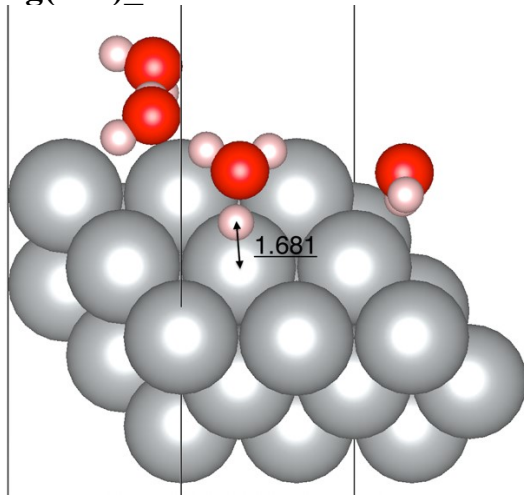
Au(111)_Volmer



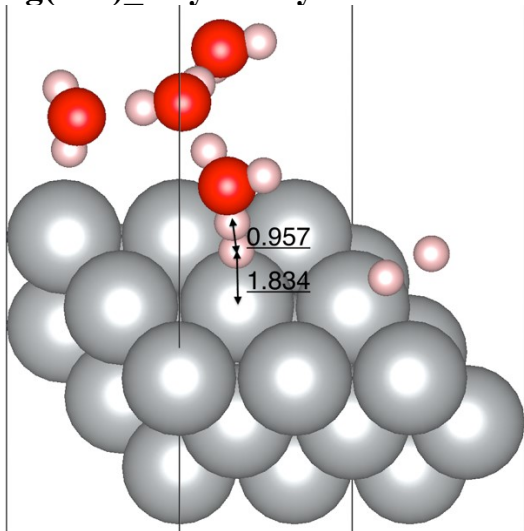
Au(111)_Heyrovsky



Ag(111)_Volmer

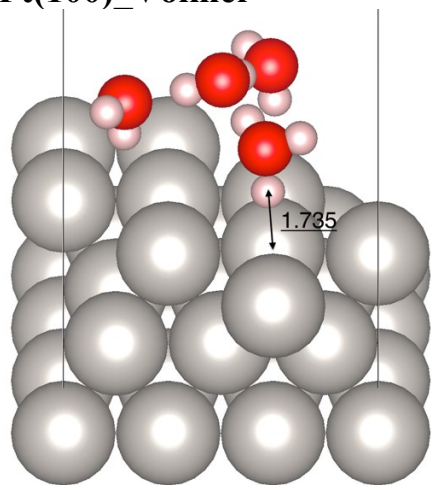


Ag(111)_Heyrovsky

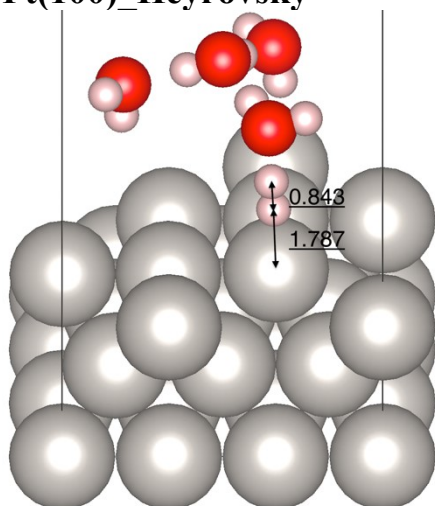


Metal(100)

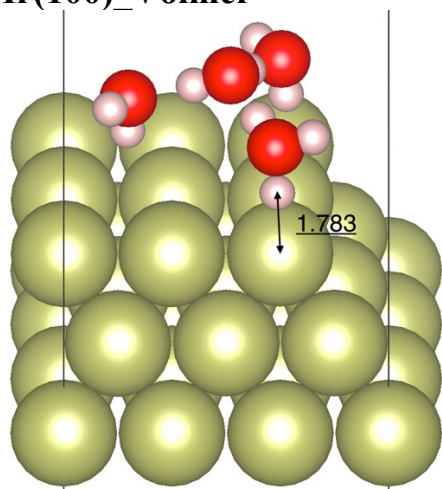
Pt(100)_Volmer



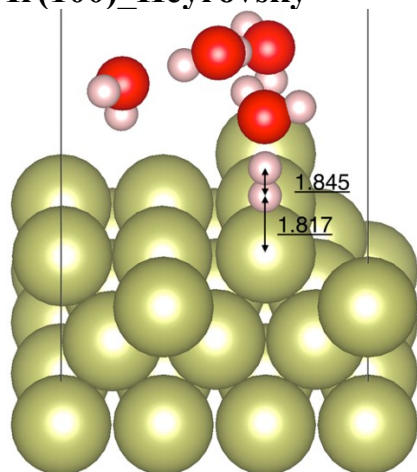
Pt(100)_Heyrovsky



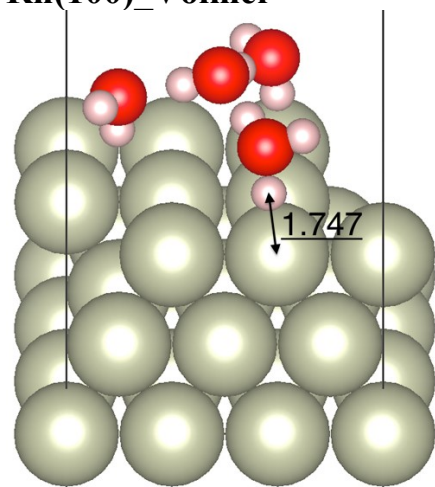
Ir(100)_Volmer



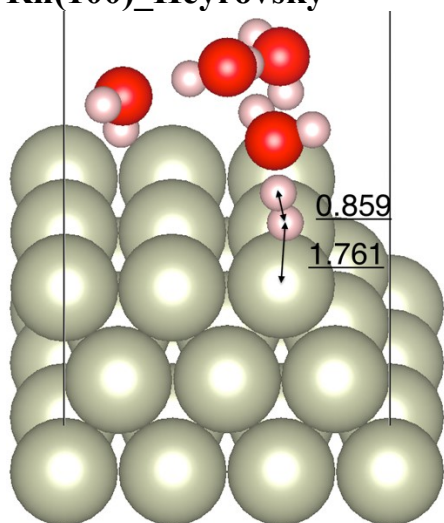
Ir(100)_Heyrovsky



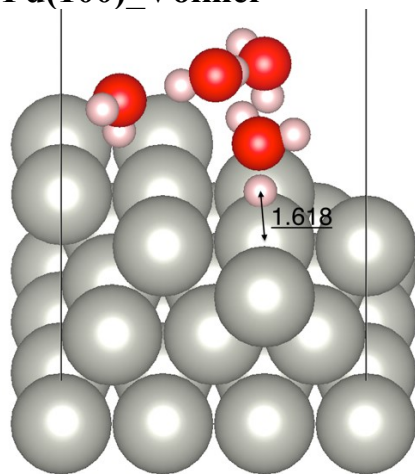
Rh(100)_Volmer



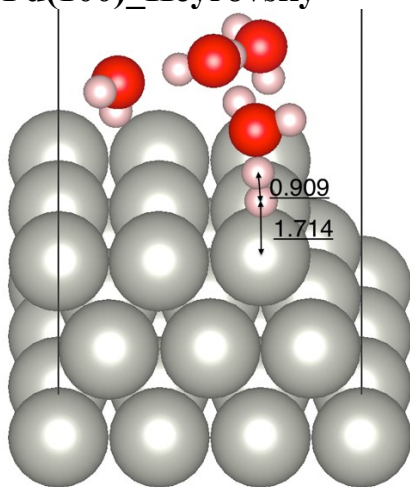
Rh(100)_Heyrovsky



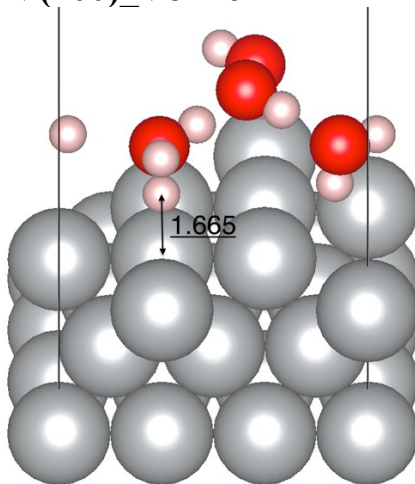
Pd(100)_Volmer



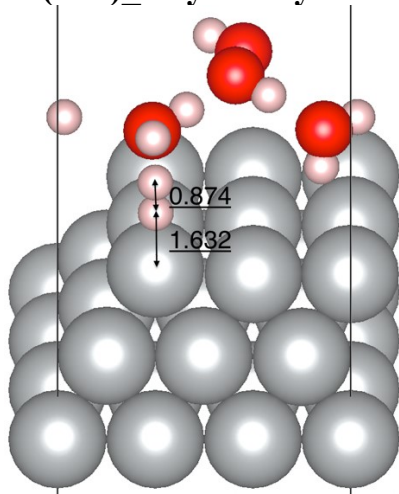
Pd(100)_Heyrovsky



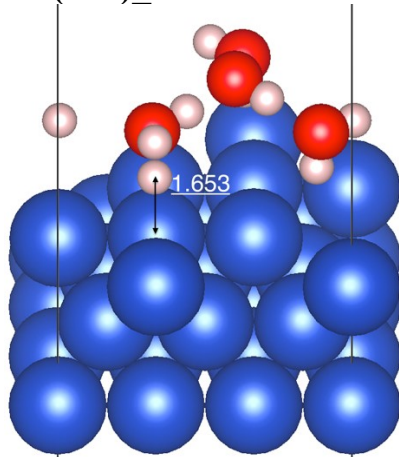
Ni(100)_Volmer



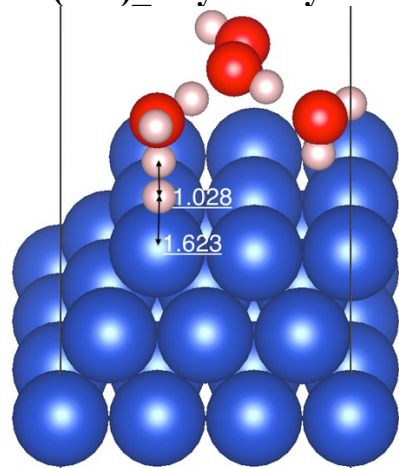
Ni(100)_Heyrovsky



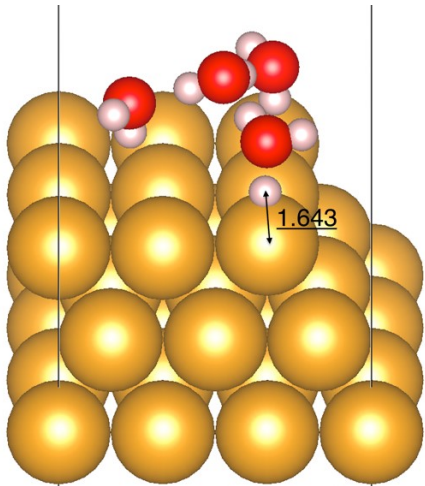
Cu(100)_Volmer



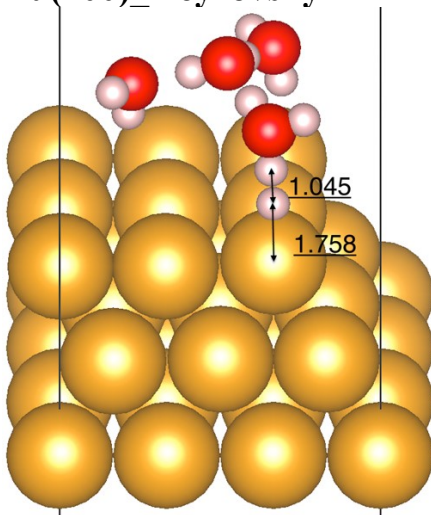
Cu(100)_Heyrovsky



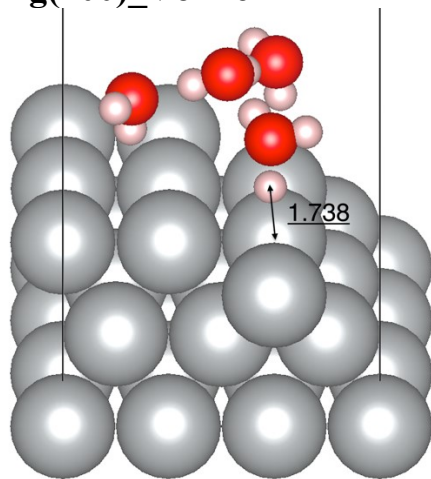
Au(100)_Volmer



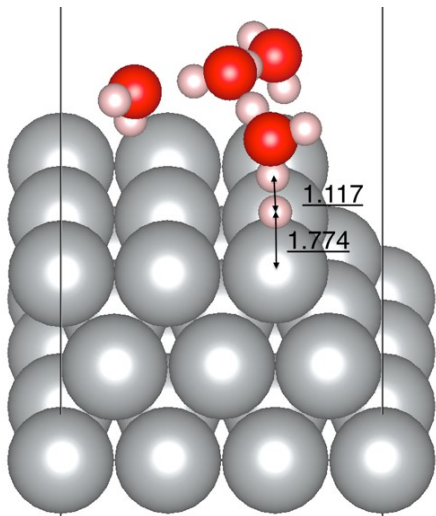
Au(100)_Heyrovsky



Ag(100)_Volmer

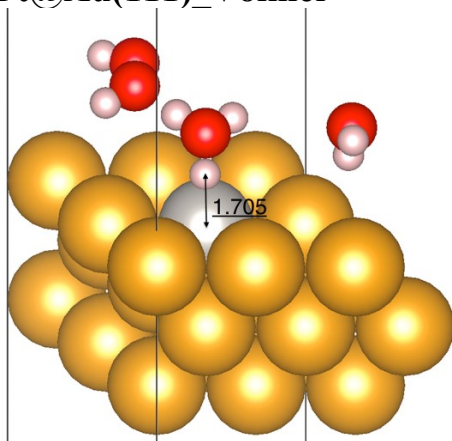


Ag(100)_Heyrovsky

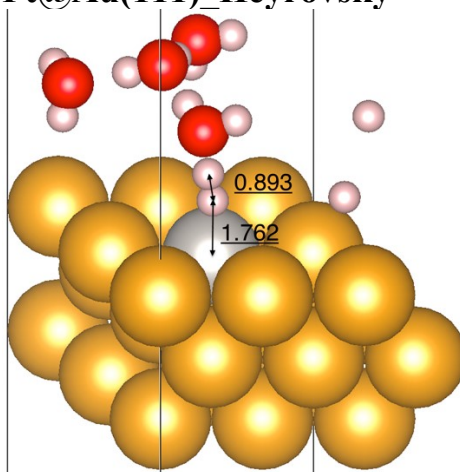


Single Atom Alloy @Au(111)

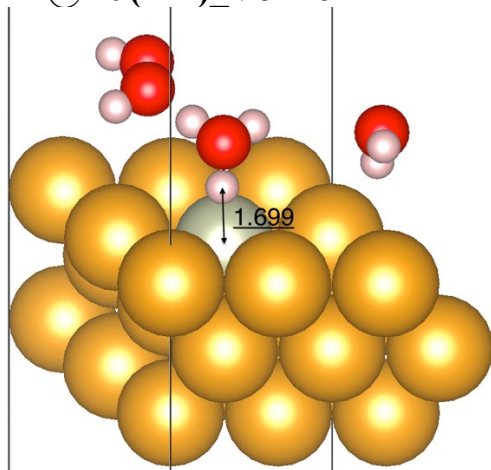
Pt@Au(111)_Volmer



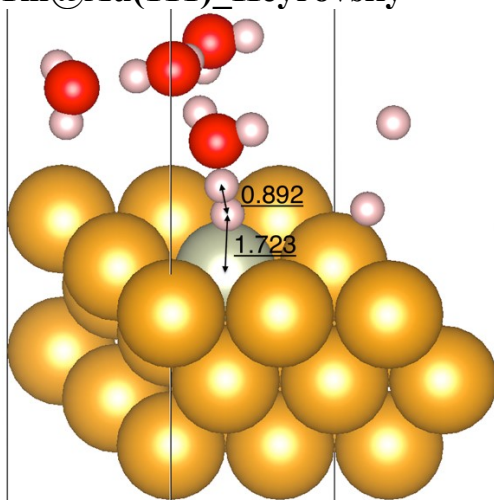
Pt@Au(111)_Heyrovsky



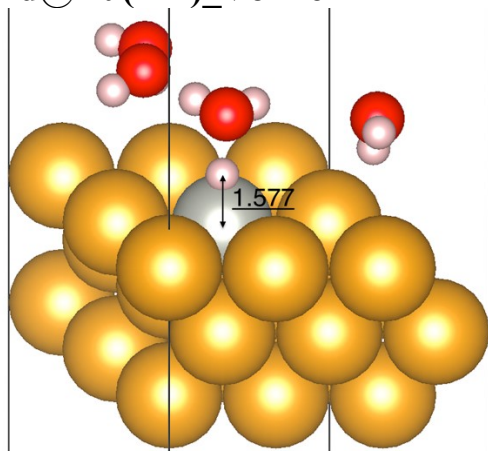
Rh@Au(111)_Volmer



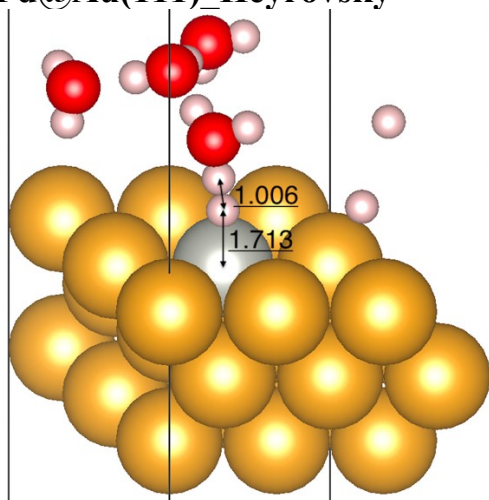
Rh@Au(111)_Heyrovsky



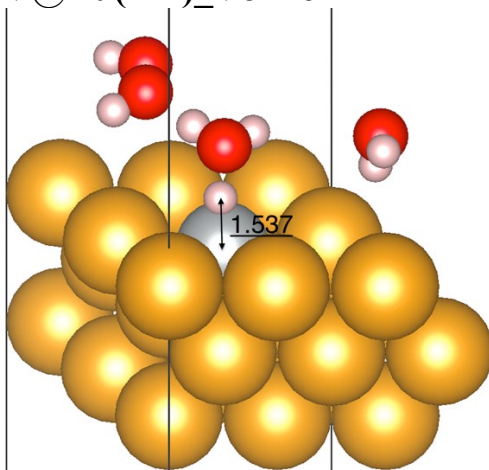
Pd@Au(111)_Volmer



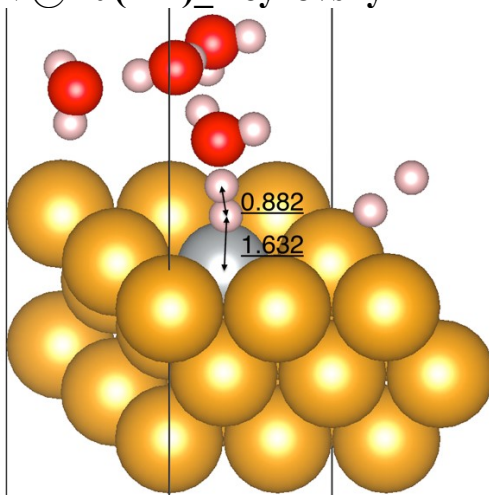
Pd@Au(111)_Heyrovsky



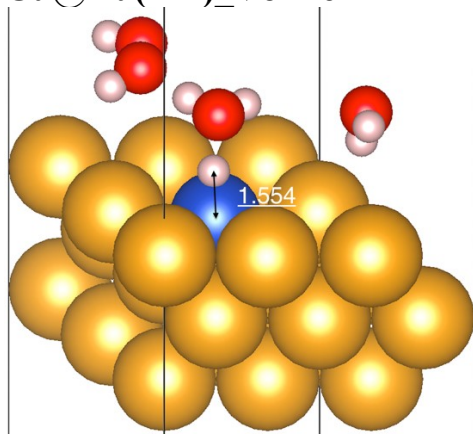
Ni@Au(111)_Volmer



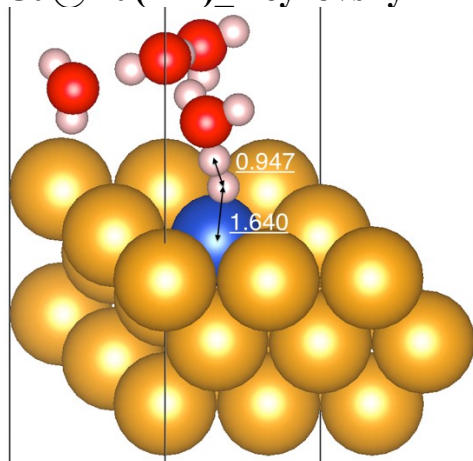
Ni@Au(111)_Heyrovsky



Cu@Au(111)_Volmer



Cu@Au(111)_Heyrovsky



4. Coordinates for Optimized Structures

Pt(111)_Rf_sur

1.0

8.3664999008	0.0000000000	0.0000000000
-4.1832499504	7.2456014549	0.0000000000
0.0000000000	0.0000000000	60.0000000000

Pt H O

27 8 4

Cartesian

0.003932484	0.329216563	29.625502825
1.396033669	1.133133431	27.291054726
0.000000000	1.932112119	24.950399995
2.790944539	0.328980734	29.624505043
4.184125200	1.130884784	27.285490036
2.788512731	1.932184458	24.950399995
5.580592551	0.328172217	29.618210793
6.974275292	1.130851206	27.285833359
5.577945530	1.932257012	24.950399995
-1.390304090	2.743574053	29.623687863
0.003901939	3.544483854	27.290870547
-1.394319075	4.347288491	24.950399995
1.397564997	2.743287938	29.651066065
2.788209657	3.544658114	27.290902734
1.394360964	4.347215937	24.950399995
4.184930260	2.743645527	29.623805881
5.579174657	3.545154766	27.285758257
4.183249950	4.347361046	24.950399995
-2.785869434	5.159133063	29.618638158
-1.392184216	5.961246274	27.285742164
-2.788805333	6.762754433	24.950399995
0.003201041	5.157478131	29.624242187
1.395997390	5.960125136	27.285679579
-0.000041640	6.762392093	24.950399995
2.791506819	5.157535138	29.624732137
4.184127382	5.961459619	27.286294699

2.788888986	6.762754433	24.950399995
1.009382004	3.386810160	34.186066389
-0.715202360	4.746565786	34.642285109
5.420912015	0.069518302	33.299124241
2.331712804	7.058617938	34.365599155
0.634584140	5.584971751	34.630694389
1.445536610	2.642232382	32.875875235
-2.551654485	4.543149559	33.326475620
-2.753848486	5.637566790	34.404959679
0.240777756	4.717763844	34.920591116
1.365858780	7.127491509	34.246727228
1.469660613	2.561948765	33.846867085
-2.419227862	4.731287036	34.274071455

Pt(111)_Rf_top

1.0

8.3664999008	0.0000000000	0.0000000000
-4.1832499504	7.2456014549	0.0000000000
0.0000000000	0.0000000000	60.0000000000

Pt H O

27 9 4

Cartesian

-0.000325795	0.320795959	29.615637660
1.395754158	1.129851640	27.300501466
0.000000000	1.932112119	24.950399995
2.795285927	0.320238170	29.615103006

4.183968801	1.131229958	27.282634377
2.788512731	1.932184458	24.950399995
5.580628612	0.328627139	29.623503685
6.974025888	1.131087116	27.282879353
5.577945530	1.932257012	24.950399995
-1.399735294	2.744591542	29.614636302
0.000793403	3.546378690	27.300773263
-1.394319075	4.347288491	24.950399995
1.398597644	2.743640561	29.705538154
2.791572520	3.546974241	27.299117446
1.394360964	4.347215937	24.950399995
4.195419293	2.744922571	29.613690376
5.579332615	3.546716630	27.276561856
4.183249950	4.347361046	24.950399995
-2.785731736	5.159605962	29.617513418
-1.393373947	5.960922370	27.276597619
-2.788805333	6.762754433	24.950399995
-0.002386693	5.166028323	29.615457058
1.395776972	5.960430901	27.282965183
-0.000041640	6.762392093	24.950399995
2.797333173	5.166634239	29.614638090
4.185265624	5.960987583	27.276681662
2.788888986	6.762754433	24.950399995
1.424217569	2.761924489	31.253825426
1.002351456	3.398827201	34.200782776
-0.714849044	4.745093104	34.632328749

5.420639080	0.061688741	33.298509121
2.321761600	7.050705188	34.375262260
0.635452844	5.587825990	34.621832371
1.445750544	2.643307742	32.901148796
-2.546058849	4.547517507	33.326843977
-2.738111507	5.633692902	34.415899515
0.241894056	4.718963583	34.910727739
1.361093123	7.127841757	34.252613783
1.465474674	2.568768016	33.876932859
-2.415325736	4.724767072	34.277318716

Pt(111)_Rf_fcc

1.0

8.3664999008	0.0000000000	0.0000000000
-4.1832499504	7.2456014549	0.0000000000
0.0000000000	0.0000000000	60.0000000000

Pt H O

27 9 4

Cartesian

-0.012683999	0.331352221	29.634116292
1.395645694	1.135249602	27.298607826
0.000000000	1.932112119	24.950399995
2.788475610	0.297921750	29.674540758
4.181771981	1.134747335	27.298121452
2.788512731	1.932184458	24.950399995
5.588732962	0.330861184	29.634869099

6.971729020	1.136184819	27.288799882
5.577945530	1.932257012	24.950399995
-1.394516709	2.755420936	29.658724666
-0.003792603	3.551809258	27.295567989
-1.394319075	4.347288491	24.950399995
1.355993723	2.776006739	29.662633538
2.788402771	3.547750962	27.298346758
1.394360964	4.347215937	24.950399995
4.219661235	2.774620647	29.662667513
5.580199449	3.551514506	27.295194268
4.183249950	4.347361046	24.950399995
-2.789012551	5.168841534	29.646479487
-1.394029839	5.962541889	27.296998501
-2.788805333	6.762754433	24.950399995
-0.001486073	5.168145789	29.650558233
1.392673423	5.962529364	27.290189266
-0.000041640	6.762392093	24.950399995
2.788065662	5.184180314	29.643997550
4.184523834	5.962923663	27.290026546
2.788888986	6.762754433	24.950399995
2.785442219	1.956206662	30.507488251
2.388328824	2.530871292	33.585923910
0.644762743	3.945333593	33.761687279
2.715815330	6.271215998	32.138106823
3.676678792	6.303353284	33.362882137
1.987359991	4.768756208	33.748190403

2.904402373	1.618704267	32.424273491
-1.032822812	3.830297709	32.172650099
-1.464973748	4.730962701	33.367427588
1.558745086	3.968322545	34.153289795
2.729557767	6.270352687	33.126068115
2.869106765	1.674688849	33.389518261
-1.027612081	3.882802486	33.159195185

Pt(111)_Volmer

1.0

8.3664999008	0.0000000000	0.0000000000
-4.1832499504	7.2456014549	0.0000000000
0.0000000000	0.0000000000	60.0000000000

Pt O H

27 4 9

Cartesian

0.002162037	0.329665925	29.611496329
1.393062769	1.134877544	27.295539379
0.000000000	1.932112119	24.950399995
2.787867545	0.333537194	29.617289901
4.181617265	1.132915552	27.285981774
2.788512731	1.932184458	24.950399995
5.577703607	0.329264986	29.628558755
6.970895971	1.132608492	27.284874916
5.577945530	1.932257012	24.950399995
-1.393304397	2.747782640	29.620315433

0.000065452	3.544926306	27.297615409
-1.394318950	4.347288491	24.950399995
1.390507521	2.745758891	29.742220044
2.786015704	3.547343923	27.298825979
1.394361213	4.347215937	24.950399995
4.182570870	2.746407993	29.632825255
5.575446135	3.546514946	27.283921838
4.183249950	4.347361046	24.950399995
-2.789826509	5.160284432	29.621415138
-1.395230042	5.961459187	27.282952666
-2.788805457	6.762754433	24.950399995
-0.000403683	5.159569685	29.624195695
1.392784629	5.960693047	27.285593748
-0.000041640	6.762392093	24.950399995
2.789109903	5.156135443	29.616161585
4.183204321	5.961146944	27.280570865
2.788888986	6.762754433	24.950399995
-0.825850727	3.982657656	33.643083572
1.246262183	2.716832137	32.818458080
5.211789456	2.838408284	32.862503529
-0.821845809	6.557973060	32.813215256
-0.850089178	4.920249820	33.290072680
-1.659259388	3.543983747	33.302063942
2.024882589	3.254040336	33.063769341
0.406390382	3.267029736	33.094958067
5.113074431	2.901533861	31.872600317

5.213225162	1.878823495	33.039093018
-1.733433729	6.903902132	32.865157127
-0.630723342	6.562442066	31.836436987
1.300262739	2.728938359	31.397942305

Pt(111)_Heyrovsky

1.0

8.3664999008	0.0000000000	0.0000000000
-4.1832499504	7.2456014549	0.0000000000
0.0000000000	0.0000000000	60.0000000000

Pt H O

27 10 4

Cartesian

-0.005526615	0.324010352	29.611941576
1.394493177	1.140253157	27.309195399
0.000000000	1.932112119	24.950399995
2.792863453	0.324139050	29.612304568
4.181928068	1.132450642	27.280592322
2.788512731	1.932184458	24.950399995
5.576883617	0.330667111	29.615042210
6.973103451	1.132375605	27.280722857
5.577945530	1.932257012	24.950399995
-1.404736204	2.744198323	29.609280825
0.004277696	3.544861525	27.305499315
-1.394318950	4.347288491	24.950399995
1.392718180	2.749048888	29.732111692

2.784237652	3.544766082	27.305213213
1.394361213	4.347215937	24.950399995
4.191462374	2.744420521	29.609232545
5.577479512	3.549149794	27.273285985
4.183249950	4.347361046	24.950399995
-2.789409252	5.161560613	29.610677361
-1.396108471	5.962144567	27.273581028
-2.788805457	6.762754433	24.950399995
-0.005184550	5.170781501	29.609851241
1.394100153	5.960910710	27.280327678
-0.000041640	6.762392093	24.950399995
2.792533855	5.171016007	29.608583450
4.184782401	5.962143271	27.273252010
2.788888986	6.762754433	24.950399995
1.429984331	2.818194754	31.525279284
0.788116687	3.791573087	34.255861044
-0.913939705	5.090234443	34.630690813
5.239610316	0.354939207	33.259770870
6.340050374	0.158612285	34.333130121
0.457465668	5.907834998	34.620273113
1.336886837	2.894782846	32.387162447
2.171692151	2.988819410	34.219250679
-2.717703739	4.875345981	33.288967609
-3.002728612	5.956570833	34.362870455
0.045549886	5.044142525	34.902774096
5.372855323	0.182617984	34.210306406

1.238879317	2.927529934	33.924794197
-2.600516222	5.077484733	34.235833883

Ir(111)_Rf_sur

1.0

8.2730998993	0.0000000000	0.0000000000
-4.1365499496	7.1647146808	0.0000000000
0.0000000000	0.0000000000	59.9491996765

Ir H O

27 8 4

Cartesian

-0.006676518	0.313981641	34.338975452
1.378947784	1.117334763	32.175858085
-0.000041298	1.910614382	29.999776963
2.762437252	0.313802787	34.338603834
4.136183072	1.114667834	32.166717709
2.757713856	1.910614382	29.999776963
5.519503216	0.323954519	34.337678362
6.895728234	1.115171539	32.165820823
5.515386290	1.910614382	29.999776963
-1.382723983	2.701236042	34.338053554
0.001990829	3.501636725	32.174357319
-1.378877639	4.298828979	29.999776963
1.383287568	2.713369607	34.349541555
2.756781005	3.502107975	32.173371102
1.378877515	4.298828979	29.999776963

4.138291879	2.701210419	34.338074993
5.515583906	3.502970616	32.169047469
4.136549950	4.298828979	29.999776963
-2.753949738	5.101719793	34.332572187
-1.377569281	5.891555679	32.166710563
-2.757713733	6.687043149	29.999776963
-0.001205667	5.097835343	34.338600261
1.378923375	5.890933467	32.167303722
0.000041422	6.687043149	29.999776963
2.756594731	5.097686303	34.338518076
4.136221535	5.891266993	32.167618168
2.757713856	6.687043149	29.999776963
1.001004339	3.401170586	38.835236178
-0.721804742	4.758098915	39.276010952
2.324142087	7.068024520	39.003975799
0.627201581	5.598012852	39.264469352
1.442341809	2.646544781	37.532003738
-2.558761906	4.554941705	37.964066926
-2.756617784	5.649514688	39.044303507
5.367957533	0.161709659	37.935409455
0.233563019	4.731397169	39.555742887
1.358584100	7.141563431	38.883735911
1.462070238	2.572952702	38.494519573
-2.426096979	4.741371356	38.911525082

Ir(111)_Rf_top

1.0

8.2730998993	0.0000000000	0.0000000000
-4.1365499496	7.1647146808	0.0000000000
0.0000000000	0.0000000000	59.9491996765

Ir H O

27 9 4

Cartesian

-0.020003371	0.297433576	34.331750339
1.378906239	1.134050578	32.190776406
-0.000041298	1.910614382	29.999776963
2.777440389	0.297033617	34.330803428
4.129980114	1.118139859	32.164259313
2.757713856	1.910614382	29.999776963
5.518187431	0.321826367	34.338828949
6.901734870	1.118565735	32.163862682
5.515386290	1.910614382	29.999776963
-1.405309136	2.698661996	34.330178109
0.016776395	3.493217215	32.189911680
-1.378877639	4.298828979	29.999776963
1.382948674	2.711690232	34.404862623
2.742133142	3.493744409	32.188743227
1.378877515	4.298828979	29.999776963
4.162884396	2.698253736	34.329845797
5.515712609	3.503304570	32.157034200
4.136549950	4.298828979	29.999776963
-2.755140164	5.099608456	34.324907564

-1.378267532	5.891230267	32.154965287
-2.757713733	6.687043149	29.999776963
-0.008143797	5.120942607	34.330685511
1.378882447	5.883658239	32.164384376
0.000041422	6.687043149	29.999776963
2.764930350	5.121156132	34.330596179
4.136761743	5.891198238	32.155933638
2.757713856	6.687043149	29.999776963
1.394102200	2.726406385	36.010667218
0.997398064	3.407315199	38.838123365
-0.721610209	4.757296914	39.269543368
2.320749947	7.063914588	39.007874215
0.627744008	5.599144108	39.258527036
1.441121226	2.649350287	37.539718386
-2.554871442	4.557694898	37.962151663
-2.749084525	5.647439223	39.048427038
5.367630737	0.156491719	37.934877040
0.233970825	4.732190202	39.548346258
1.355081996	7.141060366	38.884361230
1.460601001	2.576365260	38.508930493
-2.423955811	4.737734168	38.911339273

Ir(111)_Rf_fcc

1.0

8.2730998993	0.0000000000	0.0000000000
-4.1365499496	7.1647146808	0.0000000000

0.0000000000 0.0000000000 59.9491996765

Ir H O

27 9 4

Cartesian

-0.008661337	0.237839698	34.300802415
1.384738313	1.045850604	32.137392040
0.003350594	1.839110579	29.959013318
2.758920540	0.198156398	34.317936152
4.134732204	1.045658431	32.137367027
2.761105625	1.839110579	29.959013318
5.527215229	0.238767918	34.301981587
6.896000804	1.042568936	32.128173053
5.518778059	1.839110579	29.959013318
-1.378468153	2.633684589	34.298865713
0.002638413	3.430689795	32.127815728
-1.375485623	4.227324963	29.959013318
1.322829797	2.660711106	34.315849374
2.759962584	3.427214460	32.142215929
1.382269408	4.227324963	29.959013318
4.192737712	2.658297845	34.318429261
5.515730484	3.430537552	32.128219506
4.139941842	4.227324963	29.959013318
-2.772789666	5.027908850	34.295421099
-1.376793241	5.822401293	32.130849418
-2.754321717	6.615539132	29.959013318
0.017107645	5.027082081	34.295824876

1.381971074	5.821813245	32.127386938
0.003433314	6.615539132	29.959013318
2.758699347	5.048197155	34.300881026
4.137508072	5.821076156	32.126615116
2.761105749	6.615539132	29.959013318
2.756792717	1.841469819	35.275574500
2.414575712	2.450533189	38.315832023
0.631046400	3.894873585	38.429275587
3.717592882	6.235688163	38.089848925
1.986877438	4.709343866	38.399817708
3.009261957	1.518736930	37.210164616
-1.209786101	3.725714274	37.021253995
-1.477818734	4.756816910	38.149186327
2.666192665	6.455618627	36.970006433
1.563756999	3.891849642	38.771893162
2.755368353	6.283065975	37.935848964
2.920282343	1.598261699	38.170282800
-1.111886465	3.866119009	37.990598312

Ir(111)_Volmer

1.0

8.2730998993	0.0000000000	0.0000000000
-4.1365499496	7.1647146808	0.0000000000
0.0000000000	0.0000000000	59.9491996765

Ir O H

27 4 9

Cartesian

0.053062907	0.283759613	34.336395565
1.378462004	1.128692912	32.160600304
-0.000041298	1.910614382	29.999776963
2.760625978	0.382168517	34.335881017
4.133416141	1.118722356	32.153393057
2.757714102	1.910614382	29.999776963
5.461979866	0.288663912	34.334147991
6.899831384	1.120902661	32.188811119
5.515386783	1.910614382	29.999776963
-1.385967079	2.775107198	34.340619148
0.009908780	3.498797054	32.165549256
-1.378877639	4.298828979	29.999776963
1.323064767	2.678453764	34.398459358
2.745015770	3.498046727	32.194681970
1.378877762	4.298828979	29.999776963
4.188234831	2.671204585	34.334662539
5.516991626	3.503855678	32.160700355
4.136549950	4.298828979	29.999776963
-2.822337055	5.062362840	34.340558402
-1.380303728	5.892794125	32.193699326
-2.757713733	6.687043149	29.999776963
0.051858951	5.075020183	34.338071420
1.379285322	5.888925477	32.156240938
0.000041422	6.687043149	29.999776963
2.752181597	5.168068886	34.334151564

4.137566507	5.895174076	32.158124041
2.757713856	6.687043149	29.999776963
-0.702358375	3.973786496	38.435928980
1.308815094	2.728384695	37.523999656
-0.705047949	6.563518857	37.651350313
5.231548822	2.845849143	37.673125703
-0.734583329	4.920762364	38.108079651
-1.553177151	3.543468434	38.126614102
2.098022395	3.267537587	37.734717826
0.469233119	3.275694247	37.856008250
-0.547104882	6.595067624	36.672504722
1.282798214	2.699612396	36.194267988
5.194460150	2.898607788	36.682188231
5.199050436	1.889051760	37.868375270
-1.603252319	6.931973563	37.763285966

Ir(111)_Heyrovsky

1.0

8.2730998993	0.0000000000	0.0000000000
-4.1365499496	7.1647146808	0.0000000000
0.0000000000	0.0000000000	59.9491996765

Ir H O

27 10 4

Cartesian

-0.007888903	0.297548452	34.331339416
1.378801761	1.127002433	32.187839194

-0.000041298	1.910614382	29.999776963
2.778268391	0.304280553	34.329652841
4.132980104	1.116491659	32.163648287
2.757714102	1.910614382	29.999776963
5.499603846	0.312320308	34.344814144
6.895299286	1.115285882	32.169279730
5.515386783	1.910614382	29.999776963
-1.398659016	2.709468930	34.331110727
0.010226469	3.496973763	32.186917296
-1.378877515	4.298828979	29.999776963
1.359992190	2.700560021	34.405034139
2.747134809	3.496820879	32.192713108
1.378877762	4.298828979	29.999776963
4.175640916	2.693896756	34.329663561
5.515344622	3.503257808	32.152564063
4.136549950	4.298828979	29.999776963
-2.776550147	5.089033837	34.324217927
-1.381279603	5.889703135	32.156669728
-2.757713733	6.687043149	29.999776963
-0.000095171	5.116062703	34.330517568
1.378688652	5.887685323	32.164287899
0.000041422	6.687043149	29.999776963
2.766517934	5.133121653	34.330303173
4.136051903	5.891411336	32.151484941
2.757713856	6.687043149	29.999776963
1.582861390	2.749249944	36.294701347

0.796636944	3.541292186	39.069934434
-0.928772457	4.903119636	39.289314164
0.410105651	5.763642165	39.274252912
1.335466367	2.703169298	37.077043159
2.157360547	2.730110405	39.046944139
-3.024894941	5.733442024	39.004061557
5.505859551	4.617243215	37.959282343
5.014920919	0.441608951	37.958860699
6.168168406	0.231062917	38.972788466
0.025665166	4.897028618	39.575996072
1.213317176	2.653232815	38.801626182
-2.632236892	4.846802381	38.897435754
5.197207634	0.197884047	38.885254543

Rh(111)_Rf_sur

1.0

8.0700998306	0.0000000000	0.0000000000
-4.0350499153	6.9889114644	0.0000000000
0.0000000000	0.0000000000	59.8386993408

Rh H O

27 8 4

Cartesian

-0.001088297	0.312617708	34.321733495
1.345031289	1.088854701	32.163783822
-0.000040285	1.863732941	30.000131053
2.691093605	0.312456860	34.321423195

4.034531621	1.088169545	32.159047292
2.690046825	1.863732941	30.000131053
5.380455299	0.311870613	34.316247965
6.725707089	1.088248797	32.158911758
5.380053246	1.863732941	30.000131053
-1.344951877	2.639999301	34.321144995
0.000622554	3.417370410	32.163644722
-1.345043615	4.193347045	30.000131053
1.345010185	2.642137980	34.328431691
2.689373885	3.417313756	32.163644722
1.345043495	4.193347045	30.000131053
4.034979567	2.640145935	34.320617129
5.380140790	3.417086725	32.161754390
4.035049915	4.193347045	30.000131053
-2.689926947	4.971863517	34.317243064
-1.344388472	5.747540638	32.161522557
-2.690046705	6.522960733	30.000131053
0.000893967	4.971980574	34.322107995
1.344995394	5.746411312	32.159125758
0.000040405	6.522960733	30.000131053
2.689109086	4.971886845	34.321811962
4.034536431	5.747580212	32.161551090
2.690046825	6.522960733	30.000131053
0.939205964	3.364115065	38.835372283
-0.785108220	4.722390876	39.280092536
6.295510301	0.045128821	39.003340777

0.564721018	5.561019877	39.268440243
1.380054444	2.609443567	37.531720771
5.445443205	4.516163780	37.964603265
-2.821712324	5.612601437	39.043023485
5.202496680	0.305977349	37.935691883
0.171000506	4.693497054	39.557554061
5.331499164	0.110624581	38.883276152
1.400620860	2.536680800	38.494923464
-2.484812241	4.707823367	38.910496935

Rh(111)_Rf_top

1.0

8.0700998306	0.0000000000	0.0000000000
-4.0350499153	6.9889114644	0.0000000000
0.0000000000	0.0000000000	59.8386993408

Rh H O

27 9 4

Cartesian

-0.006559081	0.308709303	34.317696031
1.345002549	1.100935693	32.168288519
-0.000040285	1.863732941	30.000131053
2.696492763	0.308608155	34.317496298
4.030735989	1.090280625	32.158469492
2.690046825	1.863732941	30.000131053
5.380412564	0.311523062	34.308875670
6.729455582	1.090357587	32.158394592

5.380053246	1.863732941	30.000131053
-1.352064517	2.637228892	34.317460631
0.010561415	3.411216815	32.166387487
-1.345043615	4.193347045	30.000131053
1.345055641	2.644985247	34.396162648
2.679437910	3.411167034	32.166319720
1.345043495	4.193347045	30.000131053
4.041935170	2.637308041	34.317021931
5.380085353	3.415637264	32.162378556
4.035049915	4.193347045	30.000131053
-2.689985737	4.972077219	34.313544433
-1.343362106	5.748407523	32.161964823
-2.690046705	6.522960733	30.000131053
-0.000894929	4.979793791	34.318409364
1.344962685	5.741891510	32.158337525
0.000040405	6.522960733	30.000131053
2.690785184	4.979697146	34.317881497
4.033460881	5.748442515	32.161993357
2.690046825	6.522960733	30.000131053
1.339400342	2.718761741	35.975403186
0.936338751	3.369011656	38.843165444
-0.785195765	4.722014295	39.275819672
6.293029105	0.040568400	39.010299339
0.564424953	5.563382671	39.264720212
1.379757537	2.609495431	37.542484964
5.450374335	4.519991656	37.966322397

-2.813950449	5.610906407	39.050328014
5.203256564	0.298988319	37.939144414
0.170315780	4.696499702	39.555185795
5.326790159	0.112850505	38.885230684
1.399025452	2.539384975	38.512860219
-2.484500182	4.703150267	38.913164800

Rh(111)_Rf_fcc

1.0

8.0700998306	0.0000000000	0.0000000000
-4.0350499153	6.9889114644	0.0000000000
0.0000000000	0.0000000000	59.8386993408

Rh H O

27 9 4

Cartesian

-0.014667814	0.304471156	34.322264928
1.344089581	1.087774739	32.164333088
-0.000040285	1.863732941	30.000131053
2.687966178	0.275577959	34.339063917
4.034122938	1.087799317	32.164832421
2.690046825	1.863732941	30.000131053
5.391902911	0.304833183	34.323056727
6.724134950	1.086462018	32.157627759
5.380053246	1.863732941	30.000131053
-1.347052381	2.636403039	34.316461965
0.000331660	3.416568718	32.159856925

-1.345043615	4.193347045	30.000131053
1.309018325	2.660605223	34.338304218
2.689348511	3.416971959	32.165506521
1.345043495	4.193347045	30.000131053
4.066123272	2.659269278	34.340665350
5.377369300	3.416207550	32.160152958
4.035049915	4.193347045	30.000131053
-2.694247714	4.972161366	34.316258665
-1.345640796	5.748866585	32.160252824
-2.690046705	6.522960733	30.000131053
0.001259779	4.972048892	34.317414264
1.344552378	5.746988680	32.160548857
0.000040405	6.522960733	30.000131053
2.688674248	4.985203806	34.324048260
4.033922175	5.746802889	32.160131558
2.690046825	6.522960733	30.000131053
2.685048233	1.867478544	35.265101967
2.375969842	2.470333861	38.247439753
0.630005876	3.861231183	38.571242949
3.683089720	6.195899551	38.227462866
1.973096689	4.696887530	38.552314661
2.875212153	1.637245678	37.021138493
-1.174344646	3.699235658	37.136933820
-1.435198053	4.723626010	38.273051970
2.636916266	6.387804082	37.096544912
1.570251795	3.855849495	38.894290012

2.721893895	6.246005614	38.064623235
2.856591625	1.628183892	37.988332283
-1.085174787	3.827603442	38.105907376

Rh(111)_Volmer

1.0

8.0700998306	0.0000000000	0.0000000000
-4.0350499153	6.9889114644	0.0000000000
0.0000000000	0.0000000000	59.8386993408

Rh O H

27 4 9

Cartesian

-0.009922326	0.314760969	34.314707166
1.339104157	1.097439512	32.154011162
-0.000040285	1.863732941	30.000131053
2.683401883	0.322899138	34.308105270
4.028330551	1.089538086	32.151097197
2.690046825	1.863732941	30.000131053
5.374334739	0.312391536	34.307837770
6.724927183	1.091175942	32.157210460
5.380053246	1.863732941	30.000131053
-1.351856658	2.639067014	34.320827562
0.002195354	3.413839758	32.160409758
-1.345043736	4.193347045	30.000131053
1.337000196	2.641713702	34.377198693
2.677773236	3.415753279	32.154157395

1.345043495	4.193347045	30.000131053
4.017227572	2.634427448	34.310537735
5.375694284	3.416870941	32.167739253
4.035049915	4.193347045	30.000131053
-2.696641156	4.971938500	34.319201163
-1.348418540	5.747510228	32.166761987
-2.690046825	6.522960733	30.000131053
-0.003356766	4.971009129	34.318894430
1.340934902	5.742976679	32.158886792
0.000040405	6.522960733	30.000131053
2.679064522	4.973017421	34.315748632
4.030573105	5.747792247	32.165813254
2.690046825	6.522960733	30.000131053
-0.773616882	3.982165664	38.298739088
1.314705731	2.699190375	37.503529856
-0.748590130	6.595277560	37.502673856
4.936618225	2.827511919	37.537416734
-0.810420334	4.922370231	37.963436966
-1.613588670	3.540094899	37.990094215
2.092166167	3.268847435	37.672404282
0.479084638	3.251364551	37.776689983
-0.539710380	6.572072024	36.529206303
1.286988660	2.657387833	36.067865394
4.926907125	2.934718074	36.549026257
4.890281046	1.860266857	37.673545615
-1.652285850	6.966139579	37.541343632

Rh(111)_Heyrovsky

1.0

8.0700998306	0.0000000000	0.0000000000
-4.0350499153	6.9889114644	0.0000000000
0.0000000000	0.0000000000	59.8386993408

Rh H O

27 10 4

Cartesian

-0.012124761	0.297731184	34.313858300
1.343954296	1.100199195	32.174590815
-0.000040285	1.863732941	30.000131053
2.699249898	0.298091467	34.313077200
4.032779823	1.088573515	32.158045059
2.690046825	1.863732941	30.000131053
5.378951299	0.311447975	34.315092366
6.725851695	1.088591532	32.158073592
5.380053246	1.863732941	30.000131053
-1.364081876	2.638648152	34.312456601
0.008862469	3.411754817	32.172340250
-1.345043736	4.193347045	30.000131053
1.340339765	2.642253370	34.393430583
2.678951964	3.411629637	32.172044217
1.345043495	4.193347045	30.000131053
4.050634575	2.638783121	34.311746835
5.379183089	3.416675152	32.149581364

4.035049915	4.193347045	30.000131053
-2.691173048	4.971701055	34.305997371
-1.345192490	5.747734760	32.148818098
-2.690046825	6.522960733	30.000131053
-0.008407909	4.988139802	34.312670601
1.344223845	5.745336557	32.157563559
0.000040405	6.522960733	30.000131053
2.695867834	4.987719065	34.312124901
4.033588590	5.747751423	32.149103431
2.690046825	6.522960733	30.000131053
1.437889455	2.750298709	36.196308113
0.767226591	3.528560031	38.905239672
-0.947065395	4.878875575	39.207532315
0.400792642	5.727113217	39.184003029
1.294894510	2.691688545	37.022144292
2.135458518	2.713610833	38.884913251
-3.039086716	5.746376320	38.973163229
5.257407057	4.618865338	37.932974085
4.884364256	0.604848091	37.917152361
6.028259047	0.412556694	38.946666479
0.018005851	4.849045300	39.456581791
1.198314307	2.650582511	38.606652793
-2.652908751	4.857675414	38.864865031
5.061913381	0.339705145	38.838339747

Pd(111)_Rf_sur

1.0

8.2524003983	0.0000000000	0.0000000000
-4.1262001991	7.1467883871	0.0000000000
0.0000000000	0.0000000000	59.9379005432

Pd H O

27 8 4

Cartesian

0.001024835	0.318560013	34.602114984
1.375526275	1.112446741	32.300878633
-0.000041195	1.905833978	30.000117436
2.750143292	0.318448672	34.601761299
4.125861416	1.111598398	32.299267401
2.750813987	1.905833978	30.000117436
5.502071406	0.316984546	34.595880836
6.877592393	1.111719590	32.299424594
5.501586657	1.905833978	30.000117436
-1.373893767	2.699526431	34.601325444
0.000985115	3.493441673	32.301414520
-1.375427653	4.288073203	30.000117436
1.375321037	2.699753692	34.615737221
2.749805385	3.493288319	32.301385939
1.375427530	4.288073203	30.000117436
4.125093958	2.699461895	34.599807099
5.501779228	3.493149023	32.300071231
4.126200199	4.288073203	30.000117436
-2.750642259	5.082282585	34.596781126

-1.374435036	5.876298571	32.300628553
-2.750813864	6.670312001	30.000117436
0.000687158	5.080806132	34.603640474
1.375417200	5.875263009	32.299674675
0.000041318	6.670312001	30.000117436
2.750271196	5.080807410	34.602843790
4.125563459	5.876298145	32.300557101
2.750813987	6.670312001	30.000117436
0.952399078	3.461469823	39.052124377
-0.775353011	4.831308175	39.510836153
6.403902096	0.000531037	39.213833515
0.576585338	5.663958154	39.497828400
1.390580797	2.709836894	37.745900813
-2.620426064	4.616683218	38.186242397
-2.826415574	5.722785386	39.252710300
5.302993832	0.263861024	38.156189877
0.181015058	4.797565306	39.786771304
5.438428871	0.058446777	39.099207373
1.413137617	2.635763561	38.708792556
-2.477476296	4.821394727	39.128902635

Pd(111)_Rf_top

1.0

8.2524003983	0.0000000000	0.0000000000
-4.1262001991	7.1467883871	0.0000000000
0.0000000000	0.0000000000	59.9379005432

Pd H O

27 9 4

Cartesian

-0.001814166	0.313240300	34.601218267
1.375284638	1.112962179	32.308230997
-0.000041195	1.905833978	30.000117436
2.752349472	0.313184656	34.598813922
4.125422166	1.111682742	32.297131000
2.750813987	1.905833978	30.000117436
5.502027967	0.317104087	34.599303365
6.878218620	1.111981036	32.296755879
5.501586657	1.905833978	30.000117436
-1.379361413	2.699823127	34.599010414
0.000870384	3.493323889	32.305137145
-1.375427653	4.288073203	30.000117436
1.375622807	2.698786288	34.636772556
2.750325180	3.493631874	32.303508050
1.375427530	4.288073203	30.000117436
4.129926816	2.700048685	34.596763263
5.501865554	3.492787365	32.300006925
4.126200199	4.288073203	30.000117436
-2.750845283	5.082383968	34.598771051
-1.374304196	5.876439997	32.299713973
-2.750813864	6.670312001	30.000117436
-0.002544257	5.084785654	34.602257887
1.375352764	5.875139475	32.297206024

0.000041318	6.670312001	30.000117436
2.753219533	5.084723886	34.600828856
4.125224798	5.876728813	32.299781852
2.750813987	6.670312001	30.000117436
1.412003707	2.770623217	36.179918727
0.948253133	3.471942372	39.071205512
-0.776748847	4.829678795	39.503483789
2.271541973	7.139179074	39.228573968
0.573043792	5.670174080	39.492180155
1.392970111	2.704362176	37.776707146
-2.613171601	4.623881458	38.188289483
-2.811532226	5.719183710	39.267997359
5.304736169	0.252317610	38.159958946
0.178569178	4.804224254	39.784359814
5.432367189	0.058957496	39.105527262
1.409636282	2.641322836	38.743032137
-2.474228710	4.813557089	39.133739905

Pd(111)_Rf_fcc

1.0

8.2524003983	0.0000000000	0.0000000000
-4.1262001991	7.1467883871	0.0000000000
0.0000000000	0.0000000000	59.9379005432

Pd H O

27 9 4

Cartesian

-0.009482843	0.318354557	34.617477066
1.375628217	1.114275055	32.311217672
-0.000041195	1.905833978	30.000117436
2.750421620	0.297245562	34.646079120
4.126427387	1.114327557	32.310660350
2.750813987	1.905833978	30.000117436
5.510651370	0.318275138	34.618016525
6.876888695	1.115543735	32.304994242
5.501586657	1.905833978	30.000117436
-1.375907268	2.703971764	34.622410795
-0.001627267	3.497177959	32.313443388
-1.375427653	4.288073203	30.000117436
1.351990980	2.719604656	34.640177222
2.751145515	3.495142618	32.307716546
1.375427530	4.288073203	30.000117436
4.149501728	2.719258759	34.637312015
5.503676169	3.497822469	32.313446960
4.126200199	4.288073203	30.000117436
-2.750833586	5.088078919	34.620567345
-1.375348337	5.878508138	32.314207919
-2.750813864	6.670312001	30.000117436
-0.000080177	5.088008206	34.620553055
1.374473526	5.878331356	32.306366112
0.000041318	6.670312001	30.000117436
2.751021561	5.097425385	34.619909991
4.128090499	5.877860220	32.307077055

2.750813987	6.670312001	30.000117436
2.752739457	1.912371946	35.446368581
2.265234578	2.556972266	38.570948235
0.514437353	3.975996818	38.692991047
3.533297926	6.378405429	38.220514130
1.856138544	4.799489040	38.666078822
2.786851370	1.639642754	37.407356245
-1.104068124	3.907429513	37.022964794
-1.623352230	4.711919113	38.252238616
2.605666920	6.270950246	36.971573270
1.420251697	4.020556643	39.109135565
2.600185886	6.263361806	37.962402568
2.736733760	1.693700801	38.371798487
-1.108202510	3.919204501	38.011779158

Pd(111)_Volmer

1.0

8.2524003983	0.0000000000	0.0000000000
-4.1262001991	7.1467883871	0.0000000000
0.0000000000	0.0000000000	59.9379005432

Pd O H

27 4 9

Cartesian

-0.007061296	0.317318729	34.591518720
1.368478844	1.114676755	32.295476897
-0.000041195	1.905833978	30.000117436

2.742506264	0.321238134	34.571451553
4.122812919	1.111688387	32.286452566
2.750813987	1.905833978	30.000117436
5.494064053	0.317666144	34.594569701
6.874315295	1.113064308	32.296770169
5.501587149	1.905833978	30.000117436
-1.380878513	2.699949857	34.595398539
-0.004169679	3.493020377	32.299867594
-1.375427653	4.288073629	30.000117436
1.367170686	2.698703860	34.663563313
2.742687615	3.495741548	32.296330742
1.375427530	4.288073629	30.000117436
4.113639516	2.698685756	34.579257634
5.498308636	3.493075541	32.295705541
4.126199953	4.288073629	30.000117436
-2.757709227	5.082028274	34.593715855
-1.377922106	5.875087931	32.293626301
-2.750813987	6.670312427	30.000117436
-0.005489396	5.079399540	34.594573273
1.371245308	5.874504336	32.297859806
0.000041318	6.670312427	30.000117436
2.744251552	5.080475144	34.593280000
4.120942725	5.876956713	32.297066693
2.750814233	6.670312427	30.000117436
-0.797374295	4.056867756	38.554071380
1.439661829	2.741496925	37.972784477

-0.736520573	6.635482027	37.627094755
5.148808706	2.867358568	37.664156672
-0.799708149	4.975217175	38.165960875
-1.603255125	3.606971782	38.177618195
2.169712809	3.388701485	37.990654509
0.593930306	3.278092546	38.139245143
-0.529157396	6.611460488	36.652595708
1.376588001	2.656498011	36.227712666
5.095779342	2.963997860	36.673470277
5.132408274	1.901765426	37.808424487
-1.637454716	7.012536394	37.661162852

Pd(111)_Heyrovsky

1.0

8.2524003983	0.0000000000	0.0000000000
-4.1262001991	7.1467883871	0.0000000000
0.0000000000	0.0000000000	59.9379005432

Pd H O

27 10 4

Cartesian

-0.004559725	0.311809773	34.590954252
1.375638670	1.122390008	32.317162441
-0.000041195	1.905833978	30.000117436
2.754983328	0.311745130	34.590964970
4.127862389	1.111227794	32.293612011
2.750813987	1.905833978	30.000117436

5.502127803	0.319067038	34.593787306
6.875864291	1.111438655	32.293526269
5.501587149	1.905833978	30.000117436
-1.384312091	2.700722588	34.590150422
0.007563168	3.490591003	32.314993886
-1.375427653	4.288073629	30.000117436
1.374199548	2.703000526	34.687974733
2.744061440	3.490680885	32.312293018
1.375427530	4.288073629	30.000117436
4.134322391	2.700917475	34.588739254
5.502012872	3.494990116	32.290871844
4.126199953	4.288073629	30.000117436
-2.750646118	5.084150941	34.592686952
-1.375464298	5.876790580	32.290932578
-2.750813987	6.670312427	30.000117436
-0.004903074	5.091989006	34.592072469
1.375383260	5.878304519	32.293601293
0.000041318	6.670312427	30.000117436
2.755315932	5.091484217	34.589393036
4.127043530	5.877025722	32.290561030
2.750814233	6.670312427	30.000117436
1.447831118	2.779459357	36.427523340
0.828808344	3.668351497	39.095791989
-0.853761979	4.927901675	39.472045109
0.494429832	5.783953388	39.447251423
1.358725082	2.805801644	37.298228300

2.188469477	2.806237850	39.080812172
-2.929356819	5.786119079	39.264364047
-2.697335414	4.684859898	38.197070878
5.046921531	0.489378043	38.194177091
6.181362055	0.307308823	39.237055267
0.115111560	4.900414774	39.714715993
1.261180083	2.788076542	38.763538730
-2.539005432	4.901852037	39.134132888
5.217524614	0.222472474	39.115805567

Ni(111)_Rf_sur

1.0

7.4579000473	0.0000000000	0.0000000000
-3.7289500237	6.4587308998	0.0000000000
0.0000000000	0.0000000000	59.5055007935

Ni H O

27 8 4

Cartesian

-0.000284427	0.285485189	34.010600213
1.243105456	1.005210835	32.007326165
-0.000037229	1.722349696	30.000292505
2.486321918	0.286153113	34.010369671
3.728833947	1.004521738	32.003364385
2.485979203	1.722349696	30.000292505
4.972094612	0.285369746	34.006258925
6.215629632	1.004378336	32.003130296

4.971921066	1.722349696	30.000292505
-1.243451075	2.438751627	34.010625041
0.001134540	3.156655135	32.007751782
-1.243008272	3.875238694	30.000292505
1.243203530	2.439030923	34.018662099
2.485642031	3.156863212	32.006822519
1.243008161	3.875238694	30.000292505
3.728483272	2.439186836	34.009653216
4.971663464	3.156920572	32.003917686
3.728950024	3.875238694	30.000292505
-2.486540306	4.591430624	34.007223655
-1.242488844	5.309776078	32.005531482
-2.485979092	6.028127307	30.000292505
0.000569437	4.591540726	34.013331252
1.243360892	5.309040785	32.004403599
0.000037340	6.028127307	30.000292505
2.486113450	4.591009851	34.011281200
3.728731762	5.309409587	32.004375224
2.485979203	6.028127307	30.000292505
0.769730325	3.247026735	38.493171999
-0.953669969	4.603066738	38.945272495
5.816797201	0.460919046	38.669824131
0.395303843	5.442559285	38.933454543
1.207934433	2.500730123	37.184628231
4.662582673	4.397810936	37.629475512
-2.986589063	5.492735937	38.709952674

4.725756940	0.719700791	37.599544031
0.003081006	4.573874436	39.220735046
4.850910117	0.521398467	38.543724600
1.226931230	2.420252454	38.146415136
4.809017146	4.586827918	38.571872038

Ni(111)_Rf_top

1.0

7.4579000473	0.0000000000	0.0000000000
-3.7289500237	6.4587308998	0.0000000000
0.0000000000	0.0000000000	59.5055007935

Ni H O

27 9 4

Cartesian

-0.002255897	0.281500818	34.006634886
1.243299047	1.014523845	32.007510599
-0.000037229	1.722349696	30.000292505
2.487885190	0.282044541	34.006709369
3.726852030	1.005886458	32.002608916
2.485979203	1.722349696	30.000292505
4.972038838	0.285822063	34.002935569
6.217803584	1.005780783	32.002172659
4.971921066	1.722349696	30.000292505
-1.247034339	2.438808025	34.007007300
0.008635241	3.152246647	32.005123600
-1.243008272	3.875238694	30.000292505

1.243186415	2.439621853	34.072825347
2.478404156	3.152403908	32.003754533
1.243008161	3.875238694	30.000292505
3.731454036	2.439222253	34.006312127
4.971710472	3.156403365	32.006102518
3.728950024	3.875238694	30.000292505
-2.486511717	4.591921076	34.009890852
-1.241548783	5.309975108	32.007272963
-2.485979092	6.028127307	30.000292505
-0.001917905	4.593765084	34.011157061
1.243480247	5.306863778	32.003903499
0.000037340	6.028127307	30.000292505
2.487911111	4.592849240	34.009493610
3.727850268	5.309637489	32.006609711
2.485979203	6.028127307	30.000292505
1.253318151	2.532710958	35.549618867
0.765248174	3.253853030	38.507036457
-0.954255520	4.603176840	38.940480762
5.814293134	0.451705262	38.679077743
0.395369411	5.445187093	38.929138082
1.208412520	2.497310816	37.203592993
4.670313415	4.403401475	37.632231379
-2.979199980	5.491221464	38.719521952
4.727063511	0.708890630	37.604920986
0.001767656	4.577709895	39.218457998
4.849849368	0.525277621	38.553332893

1.226469479	2.424440354	38.171686116
4.805289133	4.583488300	38.580455305

Ni(111)_Rf_fcc

1.0

7.4579000473	0.0000000000	0.0000000000
-3.7289500237	6.4587308998	0.0000000000
0.0000000000	0.0000000000	59.5055007935

Ni H O

27 9 4

Cartesian

-0.011550953	0.278310569	34.001811232
1.243777801	1.004955022	32.001140539
-0.000037229	1.722349696	30.000292505
2.482540146	0.274883058	34.038073759
3.727249325	1.005135958	32.000409897
2.485979203	1.722349696	30.000292505
4.981154652	0.279017447	33.998317630
6.215367751	1.005262324	31.997146837
4.971921066	1.722349696	30.000292505
-1.246672259	2.437563609	34.002148179
0.001941687	3.155957762	32.009737992
-1.243008272	3.875238694	30.000292505
1.231580411	2.442094325	34.039691101
2.485902078	3.156099431	32.002750788
1.243008161	3.875238694	30.000292505

3.731958794	2.442079118	34.041861746
4.967291667	3.155291185	32.009982722
3.728950024	3.875238694	30.000292505
-2.489331939	4.589980826	34.004162763
-1.243698509	5.311771765	32.009862130
-2.485979092	6.028127307	30.000292505
-0.000480532	4.592130115	34.006131240
1.241991309	5.308390185	31.999203984
0.000037340	6.028127307	30.000292505
2.485330641	4.602076979	34.004240793
3.729529018	5.308477573	31.998448514
2.485979203	6.028127307	30.000292505
2.476703068	1.715245068	34.938688931
1.960765899	2.416008541	38.133799153
0.238321447	3.772490874	38.568240111
3.281192840	6.095489806	38.292142682
1.587780792	4.610333824	38.556471814
2.402209710	1.663431137	36.832405743
-1.616728041	3.564289664	37.248442333
-1.799845952	4.661175704	38.331923638
2.191419948	6.360815998	37.218024940
1.196495681	3.739481206	38.836413979
2.315992436	6.142179781	38.160534964
2.419576376	1.585572517	37.795558167
-1.450950403	3.761225102	38.188771072

Ni(111)_Volmer

1.0

7.4579000473	0.0000000000	0.0000000000
-3.7289500237	6.4587308998	0.0000000000
0.0000000000	0.0000000000	59.5055007935

Ni O H

27 4 9

Cartesian

-0.005326999	0.290592736	34.006627792
1.236044224	1.012407567	31.991791163
-0.000037229	1.722349696	30.000292505
2.474822655	0.292916369	33.977976708
3.725372038	1.004202116	31.990003573
2.485978981	1.722349696	30.000292505
4.960287084	0.289361961	34.005421879
6.212069094	1.007457137	32.004822121
4.971921066	1.722349696	30.000292505
-1.251256303	2.443308714	34.015608301
-0.001501385	3.156880921	32.000675907
-1.243008272	3.875238694	30.000292505
1.229761523	2.442689296	34.037591393
2.477096584	3.158219655	31.992426041
1.243007938	3.875238694	30.000292505
3.716411182	2.440299593	33.978522916
4.969699217	3.159088533	32.002424482
3.728950024	3.875238694	30.000292505

-2.494228277	4.591973047	34.014618742
-1.247158139	5.308492202	32.002552167
-2.485979092	6.028127307	30.000292505
-0.008369748	4.595178310	34.012487113
1.239383500	5.309150501	32.005336408
0.000037118	6.028127307	30.000292505
2.479275759	4.590537878	34.007638632
3.725415157	5.311195849	32.007840452
2.485979203	6.028127307	30.000292505
-0.915265745	3.716334478	37.908694129
1.148517935	2.377874724	37.064827824
-0.827750680	6.391021158	37.094404625
4.092895150	2.596012020	37.161350555
-0.963809262	4.659114573	37.598657330
-1.766835809	3.281564736	37.633252859
1.991073869	2.861014259	37.235202113
0.356071135	2.961363329	37.378336945
-0.673356533	6.238117475	36.118838386
1.079770624	2.413782257	35.608052467
4.175240606	2.753152686	36.181279874
3.924699043	1.622154230	37.225423574
2.041181309	0.409902052	37.123374922

Ni(111)_Heyrovsky

1.0

7.4579000473	0.0000000000	0.0000000000
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-3.7289500237	6.4587308998	0.0000000000
0.0000000000	0.0000000000	59.5055007935

Ni H O

27 10 4

Cartesian

-0.008360274	0.275870338	33.997877826
1.243301214	1.018486634	32.019775448
-0.000037229	1.722349696	30.000292505
2.492937111	0.276657458	33.997292604
3.728277957	1.005086682	31.998554918
2.485978981	1.722349696	30.000292505
4.971433589	0.286889634	34.006255378
6.216130890	1.005125468	31.998867037
4.971921066	1.722349696	30.000292505
-1.257911502	2.437849642	33.996026395
0.010563037	3.151835884	32.016913177
-1.243008272	3.875238694	30.000292505
1.240134303	2.440958855	34.092244100
2.475694773	3.152058974	32.015388051
1.243007938	3.875238694	30.000292505
3.740036823	2.438030578	33.994526096
4.971172263	3.159446748	31.992958061
3.728950024	3.875238694	30.000292505
-2.487122773	4.592510081	34.000364136
-1.244651016	5.309729112	31.993170870
-2.485979092	6.028127307	30.000292505

-0.006567642	4.605883566	33.996093784
1.243208864	5.309513529	31.998671963
0.000037118	6.028127307	30.000292505
2.491050794	4.604511532	33.995554670
3.730050669	5.309337212	31.993259540
2.485979203	6.028127307	30.000292505
1.300376841	2.533467617	35.755425730
0.667120507	3.392560545	38.419373643
-1.024708919	4.677248987	38.745605150
0.323214923	5.530864172	38.720706585
1.209207776	2.533461073	36.601778344
2.026727035	2.545447125	38.438005006
-3.100469540	5.524663069	38.539085380
4.587333844	4.437037106	37.457817281
4.495621846	0.919882732	37.452780819
5.617046592	0.745506798	38.511232326
-0.059222797	4.652730994	38.997052290
1.105225487	2.512983729	38.108687779
4.749200908	4.643032821	38.396741486
4.655798297	0.653760950	38.376588544

Cu(111)_Rf_sur

1.0

7.6687002182	0.0000000000	0.0000000000
-3.8343501091	6.6412892030	0.0000000000
0.0000000000	0.0000000000	59.6202011108

Cu H O

27 8 4

Cartesian

-0.000171052	0.291794028	34.164430065
1.278146795	1.032742208	32.080656770
-0.000038281	1.771032516	30.000287863
2.555814073	0.291414184	34.162464902
3.834286574	1.031370186	32.075042018
2.556246281	1.771032516	30.000287863
5.112865433	0.290804720	34.158307142
6.390706720	1.031260238	32.075635476
5.112454166	1.771032516	30.000287863
-1.276945119	2.504437223	34.164007182
0.001481315	3.244918570	32.081896991
-1.278142338	3.984773680	30.000287863
1.278863855	2.505106806	34.179835099
2.554441689	3.244559137	32.079953149
1.278142224	3.984773680	30.000287863
3.833257207	2.504565479	34.161189145
5.112672769	3.245017731	32.075393828
3.834350109	3.984773680	30.000287863
-2.556409205	4.718878253	34.160794691
-1.277128855	5.458193817	32.077884930
-2.556246167	6.198514448	30.000287863
0.000815677	4.716707402	34.171683046
1.277880311	5.457730274	32.078151453

0.000038396	6.198514448	30.000287863
2.555486825	4.717280595	34.166995794
3.833714525	5.458654192	32.076683800
2.556246281	6.198514448	30.000287863
0.737971137	3.343382718	38.614196156
-0.985399864	4.698941183	39.060778655
5.892208856	0.370487042	38.789952128
0.364231602	5.539472064	39.049563364
1.177368586	2.595478558	37.306847202
4.843907759	4.495512606	37.746055896
-3.018002995	5.588123819	38.829386881
4.801927514	0.629937290	37.718383694
-0.027678637	4.669256265	39.333730260
4.925855310	0.436840592	38.663634408
1.196063574	2.515895348	38.269436129
-2.683061540	4.682908002	38.691978248

Cu(111)_Rf_top

1.0

7.6687002182	0.0000000000	0.0000000000
-3.8343501091	6.6412892030	0.0000000000
0.0000000000	0.0000000000	59.6202011108

Cu H O

27 9 4

Cartesian

-0.007947984	0.280165687	34.148616363
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1.278135482	1.038338957	32.079661751
-0.000038281	1.771032516	30.000287863
2.563309895	0.279585739	34.147461430
3.831545632	1.033695023	32.071847294
2.556246281	1.771032516	30.000287863
5.112604777	0.291044804	34.149625597
6.393203175	1.033461471	32.072501164
5.112454166	1.771032516	30.000287863
-1.290274154	2.503842060	34.149433701
0.004813159	3.243190480	32.076093895
-1.278142338	3.984773680	30.000287863
1.278229871	2.503167133	34.191032621
2.551259999	3.243023826	32.074189144
1.278142224	3.984773680	30.000287863
3.845332157	2.503969326	34.147102512
5.112634145	3.245755994	32.076701568
3.834350109	3.984773680	30.000287863
-2.556465156	4.719273313	34.151608529
-1.276468474	5.457775006	32.078588551
-2.556246167	6.198514448	30.000287863
-0.004904806	4.726317097	34.159778349
1.277857000	5.454476373	32.076669585
0.000038396	6.198514448	30.000287863
2.560023217	4.726614382	34.156178511
3.833079398	5.458018059	32.077927574
2.556246281	6.198514448	30.000287863

1.286481491	2.626422284	35.713206275
0.733642722	3.350308539	38.625073850
-0.984849985	4.698503371	39.056844774
5.889141924	0.363381257	38.797912283
0.364976888	5.540792229	39.046080796
1.177702034	2.593849628	37.320763260
4.851381412	4.499647277	37.750199442
-3.009619247	5.587309552	38.838064872
4.802025931	0.620393059	37.723174002
-0.028840332	4.673136403	39.334003890
4.923938703	0.439493639	38.671484401
1.195113398	2.520499697	38.291628617
-2.684740238	4.678306622	38.698623556

Cu(111)_Rf_fcc

1.0

7.6687002182	0.0000000000	0.0000000000
-3.8343501091	6.6412892030	0.0000000000
0.0000000000	0.0000000000	59.6202011108

Cu H O

27 9 4

Cartesian

-0.015474987	0.283047883	34.148051334
1.276115200	1.028853262	32.058865844
-0.000038281	1.771032516	30.000287863
2.555601198	0.273183012	34.181057551

3.836242977	1.031374046	32.056875805
2.556246281	1.771032516	30.000287863
5.126655514	0.282703789	34.143332099
6.390643927	1.032834442	32.068229688
5.112454166	1.771032516	30.000287863
-1.276942534	2.506063580	34.151903481
0.009673513	3.239750529	32.086289291
-1.278142338	3.984773680	30.000287863
1.269405974	2.509971032	34.183957322
2.556576643	3.247715064	32.060177138
1.278142224	3.984773680	30.000287863
3.849805813	2.513261351	34.183278577
5.104690147	3.240230301	32.082181282
3.834350109	3.984773680	30.000287863
-2.554100771	4.715787839	34.152379669
-1.276975387	5.467193901	32.084452059
-2.556246167	6.198514448	30.000287863
-0.001683234	4.714991385	34.158232516
1.276374199	5.456605264	32.071587879
0.000038396	6.198514448	30.000287863
2.555663719	4.735504023	34.152244631
3.835617392	5.457412801	32.070457821
2.556246281	6.198514448	30.000287863
2.566674564	1.760234870	35.042669772
2.023334357	2.463761681	38.024938527
0.303711495	3.819797741	38.438532578

3.346136460	6.138178734	38.160300263
1.650040371	4.658664857	38.426855314
2.476377319	1.695254628	36.739423143
-1.541641955	3.619361407	37.108468752
-1.735326537	4.707129375	38.198956769
2.262421646	6.393679225	37.078788743
1.255230580	3.797244091	38.727642588
2.381492259	6.203465365	38.030411134
2.483207503	1.628241491	37.705228116
-1.401077192	3.802330785	38.059394630

Cu(111)_Volmer

1.0

7.6687002182	0.0000000000	0.0000000000
-3.8343501091	6.6412892030	0.0000000000
0.0000000000	0.0000000000	59.6202011108

Cu O H

27 4 9

Cartesian

-0.008359436	0.294928406	34.154813913
1.270085039	1.032770017	32.052497720
-0.000038167	1.771032516	30.000287863
2.545159688	0.286177189	34.106239196
3.830745953	1.030961667	32.053350594
2.556246281	1.771032516	30.000287863
5.097683912	0.291029886	34.147823901

6.386449154	1.033260477	32.076164968
5.112454166	1.771032516	30.000287863
-1.287886972	2.506498225	34.168005028
-0.008701854	3.247638863	32.056015824
-1.278142338	3.984773680	30.000287863
1.261184294	2.509146868	34.132664069
2.547450152	3.247324359	32.053016551
1.278141995	3.984773680	30.000287863
3.828950046	2.506564530	34.106548362
5.113618146	3.246006371	32.069789736
3.834350109	3.984773680	30.000287863
-2.566698633	4.715561807	34.153417332
-1.282715297	5.452404882	32.069061240
-2.556246052	6.198514448	30.000287863
-0.009029587	4.722842707	34.162660352
1.273845805	5.455726869	32.074114517
0.000038396	6.198514448	30.000287863
2.550943121	4.720419303	34.156420159
3.828646995	5.460778728	32.082039137
2.556246281	6.198514448	30.000287863
-0.822283130	3.855473082	38.030436010
1.308788976	2.476317107	37.304505352
-0.707667660	6.557211889	37.228226450
4.417495098	2.682370378	37.272941914
-0.866988489	4.794887714	37.715249383
-1.665540641	3.414547746	37.745206576

2.120805175	3.018648362	37.402152297
0.514348579	3.061966016	37.563196196
2.262956699	0.382531225	37.267263196
-0.554571255	6.414141194	36.255498985
1.158305299	2.513925788	35.704435890
4.484867787	2.826649806	36.293153364
4.239385121	1.715806258	37.356168184

Cu(111)_Heyrovsky

1.0

7.6687002182	0.0000000000	0.0000000000
-3.8343501091	6.6412892030	0.0000000000
0.0000000000	0.0000000000	59.6202011108

Cu H O

27 10 4

Cartesian

-0.009650273	0.280902688	34.139885068
1.278309176	1.039033281	32.091900490
-0.000038167	1.771032516	30.000287863
2.565269226	0.281138245	34.139138803
3.833646647	1.032644829	32.068261671
2.556246281	1.771032516	30.000287863
5.113128617	0.293215630	34.157550217
6.391657525	1.032705790	32.068919094
5.112454166	1.771032516	30.000287863
-1.296361923	2.505722751	34.135649128

0.004951772	3.244366555	32.089348976
-1.278142338	3.984773680	30.000287863
1.274908083	2.506051506	34.202240805
2.551323420	3.244042155	32.087191916
1.278141995	3.984773680	30.000287863
3.851081323	2.505420716	34.132760018
5.112619861	3.247482106	32.059484178
3.834350109	3.984773680	30.000287863
-2.556683630	4.721191214	34.139792673
-1.279622168	5.459657280	32.061076209
-2.556246052	6.198514448	30.000287863
-0.009106150	4.739556357	34.138605757
1.278117541	5.458548896	32.070205512
0.000038396	6.198514448	30.000287863
2.563556981	4.738433722	34.135755737
3.835345651	5.460118448	32.060461429
2.556246281	6.198514448	30.000287863
1.333938876	2.630414052	35.902718391
0.695605965	3.456527421	38.571143796
-0.987091441	4.754491049	38.916276955
0.359860221	5.612343213	38.894109343
1.232328192	2.612993412	36.751811136
2.057226449	2.614420061	38.562728774
4.828793616	4.508065063	37.639674102
-3.053231105	5.601983378	38.719064099
4.638432652	0.813676006	37.636617971

5.764438303	0.628426621	38.689767883
-0.018692245	4.727437754	39.157124967
1.129469538	2.578150348	38.249951516
-2.670388209	4.716587855	38.576086911
4.802008676	0.544496218	38.558251187

Au(111)_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	60.1489982605

Au H O

27 8 4

Cartesian

-0.000024382	0.333808274	34.936732118
1.439925670	1.166005620	32.470418319
-0.000043130	1.995370371	29.999915261
2.879558118	0.334252456	34.932842220
4.319303542	1.164665518	32.463477450
2.880047681	1.995370371	29.999915261
5.760588191	0.333520050	34.920745891
7.201852787	1.163859160	32.464061831
5.760052102	1.995370371	29.999915261
-1.439227859	2.827681474	34.930171276
0.002408480	3.657294756	32.469729968
-1.440045470	4.489527587	29.999915261

1.440093364	2.827459815	34.957716058
2.878372804	3.657241906	32.469726383
1.440045341	4.489527587	29.999915261
4.319463318	2.827598519	34.930615836
5.760751716	3.657484304	32.462828536
4.320049763	4.489527587	29.999915261
-2.880887436	5.323388743	34.919125399
-1.439150417	6.153299726	32.463183467
-2.880047552	6.983684356	29.999915261
-0.000239985	5.321007132	34.931953100
1.440173316	6.151153155	32.464137119
0.000043259	6.983684356	29.999915261
2.879519816	5.321451343	34.933677562
4.319135398	6.153033022	32.463068742
2.880047681	6.983684356	29.999915261
1.033418843	3.550928864	39.399574733
-0.695211737	4.919286081	39.849548124
2.359070601	7.234403273	39.564585292
0.656447534	5.755242073	39.837254611
1.472940203	2.800590878	38.094365087
-2.538559379	4.711145810	38.532016284
-2.744078524	5.812450677	39.603674288
5.580264354	0.012138329	38.503263303
0.262299116	4.886354295	40.120908860
1.393659929	7.300298065	39.448999744
1.494065224	2.724555732	39.057041407

-2.403195464 4.908426115 39.476791902

Au(111)_Rf_top

1.0

8.6400995255 0.0000000000 0.0000000000
-4.3200497627 7.4825456803 0.0000000000
0.0000000000 0.0000000000 60.1489982605

Au H O

27 9 4

Cartesian

-0.012834631 0.313300890 34.931673458
1.439932816 1.173683080 32.490817878
-0.000043130 1.995370371 29.999915261
2.892913903 0.313404835 34.930146180
4.320140530 1.163779550 32.462824951
2.880047681 1.995370371 29.999915261
5.760625029 0.333162780 34.927034261
7.200325906 1.163206113 32.462961187
5.760052102 1.995370371 29.999915261
-1.463595113 2.826465024 34.927579205
0.007945653 3.653901407 32.488749240
-1.440045470 4.489527587 29.999915261
1.439464819 2.826994197 34.934806887
2.874366053 3.654827515 32.486770232
1.440045341 4.489527587 29.999915261
4.343742138 2.825734931 34.927213519

5.760844157	3.659263376	32.455934274
4.320049763	4.489527587	29.999915261
-2.881108174	5.322552949	34.922043719
-1.440627151	6.152661508	32.456421856
-2.880047552	6.983684356	29.999915261
-0.011661692	5.342872012	34.929597650
1.440131602	6.151864962	32.463491791
0.000043259	6.983684356	29.999915261
2.890035655	5.342771217	34.929411222
4.320974427	6.152389897	32.456221087
2.880047681	6.983684356	29.999915261
1.468837019	2.862434256	36.539847022
1.026676079	3.564669062	39.410513055
-0.695013981	4.917512361	39.840760897
2.350414390	7.225612276	39.574118232
0.655316615	5.759037040	39.829546518
1.471599555	2.802908488	38.113326996
-2.529494170	4.715917505	38.529775559
-2.725684817	5.807432793	39.614246924
5.579537319	0.000906176	38.503066120
0.261462515	4.891053292	40.116979525
1.383735555	7.299632641	39.450813835
1.490178465	2.733111021	39.082639447
-2.396328297	4.899073611	39.478028782

Au(111)_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	60.1489982605

Au H O

27 9 4

Cartesian

-0.005624898	0.333222544	34.890809808
1.442025092	1.166762138	32.440328074
-0.000043130	1.995370371	29.999915261
2.878765420	0.259247558	34.952614375
4.317173028	1.166479824	32.439682745
2.880047681	1.995370371	29.999915261
5.762556209	0.331140697	34.902952744
7.199088063	1.168545224	32.451259226
5.760052102	1.995370371	29.999915261
-1.440027542	2.829424866	34.962337329
0.000295733	3.656760455	32.463086668
-1.440045470	4.489527587	29.999915261
1.367564867	2.866808347	34.952628716
2.879235928	3.653414381	32.444813109
1.440045341	4.489527587	29.999915261
4.387338107	2.864120784	34.953231023
5.759352231	3.655385900	32.459971164
4.320049763	4.489527587	29.999915261
-2.881266775	5.321944167	34.927966403

-1.440977473	6.156205826	32.456991896
-2.880047552	6.983684356	29.999915261
-0.000867758	5.321752389	34.930515451
1.437862813	6.152719933	32.449653074
0.000043259	6.983684356	29.999915261
2.878107456	5.325319453	34.893132991
4.321415259	6.150747746	32.449459476
2.880047681	6.983684356	29.999915261
2.878596439	2.003745702	35.605411005
2.453553510	2.673757853	38.638811020
0.709598113	4.077086612	38.913025543
3.774746355	6.398167196	38.595652868
2.059029150	4.898984412	38.897372736
2.955894130	1.824180743	37.427790689
-1.109256023	3.883928634	37.524640193
-1.366146971	4.940489996	38.629650937
2.705723544	6.613851463	37.496009108
1.636533620	4.081582682	39.266887973
2.814182254	6.491049114	38.464213744
2.938267565	1.831102578	38.390262656
-1.046221625	4.030015463	38.494339841

Au(111)_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000

0.0000000000 0.0000000000 60.1489982605

Au O H

27 4 9

Cartesian

-0.012753359	0.317934048	34.903146342
1.437099276	1.171954071	32.462455679
-0.000043130	1.995370371	29.999917054
2.883863741	0.318821856	34.877039210
4.320026588	1.162882432	32.440736782
2.880047681	1.995370371	29.999917054
5.756523213	0.327801787	34.905867478
7.200027920	1.160382633	32.449495327
5.760052102	1.995370371	29.999917054
-1.458449235	2.822444830	34.901084875
0.011195369	3.647631394	32.473268521
-1.440045341	4.489527587	29.999917054
1.433484754	2.816951739	34.998845009
2.865568993	3.649913547	32.475150730
1.440045599	4.489527587	29.999917054
4.328832661	2.826791938	34.895298428
5.759979360	3.654733187	32.442529362
4.320049763	4.489527587	29.999917054
-2.886166760	5.318017631	34.895004445
-1.441354961	6.146490729	32.439413858
-2.880047423	6.983684356	29.999917054
-0.006811774	5.328824078	34.892928637

1.441725239	6.149298264	32.447107611
0.000043517	6.983684356	29.999917054
2.880742145	5.330834621	34.914805282
4.317414044	6.148207807	32.450800325
2.880047681	6.983684356	29.999917054
-0.770401960	4.134148037	38.998857851
1.513718146	2.806210854	38.488553393
-0.743280781	6.737507892	38.101503140
5.541183772	2.940357073	38.130887109
-0.770079318	5.052735656	38.614564585
-1.576814922	3.689874430	38.620490854
2.227397813	3.470820228	38.489033805
0.665417115	3.327562119	38.649688395
-1.648872782	7.093447164	38.186030450
-0.571266117	6.749242007	37.129164814
1.430446828	2.740897639	36.602336355
5.459777361	3.013871903	37.149030184
5.566332668	1.979268633	38.300006261

Au(111)_Heyrovsky

1.0

8.6513996124	0.0000000000	0.0000000000
-4.3256998062	7.4923318427	0.0000000000
0.0000000000	0.0000000000	64.7091979980

Au H O

27 10 4

Cartesian

-0.011565174	0.320115297	34.790270914
1.442025736	1.181652504	32.386503845
0.000129947	1.998129874	29.873648199
2.895792793	0.320955812	34.789333671
4.325787791	1.166527585	32.328844090
2.883468127	1.997680394	29.873002157
5.768637912	0.332615651	34.814504249
7.209588586	1.166388141	32.327902990
5.767801796	1.997755419	29.873002157
-1.462736575	2.826565816	34.783235803
0.011743336	3.657428461	32.383684400
-1.441669219	4.495399284	29.873648199
1.440790141	2.832252537	34.912552252
2.871911719	3.657268139	32.385150049
1.441625774	4.495324259	29.873648199
4.344328412	2.828149827	34.787802454
5.766844982	3.666176696	32.315319629
4.325742864	4.495623913	29.874296170
-2.884141004	5.329401594	34.784007197
-1.443927181	6.161479601	32.315115210
-2.884203464	6.992743049	29.874296170
-0.008847498	5.348964827	34.783621500
1.442212084	6.161433603	32.328313757
-0.000000258	6.993043150	29.873648199
2.890806278	5.348265040	34.786903781

4.327608277	6.161777468	32.317107334
2.884290869	6.992743049	29.874296170
1.441302195	2.876790632	36.724679598
0.797882422	3.839143415	39.326802857
-0.865413340	5.045500043	39.676248084
5.219158494	0.259149392	38.394689217
6.353422637	0.100690792	39.445061377
0.490938047	5.900502673	39.637470120
1.351158526	2.930508133	37.667534897
2.175156602	2.948180779	39.318294384
-2.694015214	4.817714563	38.397072824
-2.954458826	5.906360434	39.471061203
0.109232763	5.014925542	39.903662676
1.069705981	7.468391701	39.310472452
1.250999895	2.945680613	38.985221990
-2.545375511	5.031165343	39.336599558

Ag(111)_Rf_sur

1.0

8.6679000854	0.0000000000	0.0000000000
-4.3339500427	7.5066216715	0.0000000000
0.0000000000	0.0000000000	60.1641006470

Ag H O

27 8 4

Cartesian

0.001720677	0.335975552	34.818521756
-------------	-------------	--------------

1.444561711	1.164743600	32.401782787
-0.000043269	2.001790716	30.000227196
2.887273954	0.335784891	34.816800447
4.333763791	1.167432651	32.404429299
2.889314581	2.001790716	30.000227196
5.779232298	0.333307782	34.807516138
7.223691697	1.167457148	32.404303787
5.778585763	2.001790716	30.000227196
-1.440903978	2.835495086	34.815452089
-0.001853601	3.671090740	32.401678791
-1.444678990	4.503973182	30.000227196
1.444319145	2.834919020	34.809276894
2.891063173	3.671038391	32.401678791
1.444678860	4.503973182	30.000227196
4.329953648	2.835651015	34.814921352
5.778630453	3.669205272	32.404547639
4.333950043	4.503973182	30.000227196
-2.889700694	5.338597019	34.811299431
-1.443827426	6.172074542	32.404863213
-2.889314452	7.006155200	30.000227196
0.001278960	5.334135252	34.819360894
1.444617379	6.171237402	32.405666490
0.000043398	7.006155200	30.000227196
2.887261425	5.334185364	34.819238968
4.333089825	6.172178346	32.405067618
2.889314581	7.006155200	30.000227196

0.969560107	3.447856968	39.260039766
-0.760845785	4.826298722	39.691995019
2.296084358	7.141046252	39.397758808
0.590808698	5.661288110	39.679716350
1.424993702	2.690910250	37.964561302
-2.610589994	4.609297196	38.367236376
-2.814166193	5.715098668	39.435939587
1.196107538	7.407691873	38.338020746
0.196601015	4.792646653	39.963258930
1.328491643	7.201843869	39.279942398
1.428980151	2.616794445	38.927278514
-2.463925049	4.813963538	39.309054032

Ag(111)_Rf_top

1.0

8.6679000854	0.0000000000	0.0000000000
-4.3339500427	7.5066216715	0.0000000000
0.0000000000	0.0000000000	60.1641006470

Ag H O

27 9 4

Cartesian

-0.008403136	0.319517696	34.808900357
1.444570623	1.169041832	32.401087092
-0.000043269	2.001790716	30.000227196
2.897284686	0.319800164	34.807817367
4.331622935	1.168800667	32.403156248

2.889314581	2.001790716	30.000227196
5.779252658	0.333636726	34.798626296
7.225864327	1.168814426	32.402941085
5.778585763	2.001790716	30.000227196
-1.459824177	2.834823046	34.806117575
0.001404376	3.669140171	32.400373466
-1.444678990	4.503973182	30.000227196
1.444375718	2.833484561	34.767631981
2.888061453	3.669252252	32.399476951
1.444678860	4.503973182	30.000227196
4.348182250	2.834793292	34.806350669
5.778570780	3.670693870	32.404877557
4.333950043	4.503973182	30.000227196
-2.889736714	5.339010892	34.802900879
-1.444822101	6.171389975	32.404436471
-2.889314452	7.006155200	30.000227196
-0.007085298	5.349972467	34.810083757
1.444692552	6.168826204	32.404328890
0.000043398	7.006155200	30.000227196
2.895505046	5.349880297	34.810478224
4.334168843	6.171324203	32.404605016
2.889314581	7.006155200	30.000227196
1.456068862	2.874923470	36.431535061
0.970552845	3.450678011	39.268273359
-0.762387460	4.827538997	39.687792156
2.290789242	7.136160321	39.404202958

0.586824832	5.667097982	39.676069327
1.425111497	2.691028819	37.970065904
-2.604462285	4.613741513	38.366314759
-2.803295389	5.712850335	39.443667546
1.196409519	7.399838143	38.337117059
0.192279778	4.801727235	39.968161074
1.325789578	7.202477430	39.283919338
1.427127842	2.615134706	38.945079715
-2.461959401	4.808266865	39.310821959

Ag(111)_Rf_fcc

1.0

8.6679000854	0.0000000000	0.0000000000
-4.3339500427	7.5066216715	0.0000000000
0.0000000000	0.0000000000	60.1641006470

Ag H O

27 9 4

Cartesian

-0.017274387	0.326647206	34.806917266
1.440222715	1.169120467	32.383891935
-0.000043269	2.001790716	30.000227196
2.888866583	0.299995340	34.815495121
4.338344191	1.168335005	32.381636303
2.889314581	2.001790716	30.000227196
5.793414165	0.325403660	34.810008450
7.222607319	1.169888368	32.403887804

5.778585763	2.001790716	30.000227196
-1.445292556	2.844461126	34.811851685
0.007016843	3.668290950	32.409969762
-1.444678990	4.503973182	30.000227196
1.410431099	2.855930534	34.838575003
2.888421427	3.674659214	32.387148077
1.444678860	4.503973182	30.000227196
4.366041190	2.856332549	34.827730758
5.772095384	3.668177079	32.406900095
4.333950043	4.503973182	30.000227196
-2.883236518	5.336162555	34.814516127
-1.444048293	6.180437448	32.406193641
-2.889314452	7.006155200	30.000227196
-0.005975024	5.336251146	34.819916733
1.443341519	6.173381931	32.406473353
0.000043398	7.006155200	30.000227196
2.889413260	5.357512550	34.806275361
4.335196196	6.173433833	32.405117823
2.889314581	7.006155200	30.000227196
2.894475110	2.000012183	35.649393892
2.410281322	2.609154139	38.621513121
0.661250172	4.032989184	38.883270388
3.740612874	6.358368981	38.537746350
2.013383328	4.856243838	38.864009660
2.918415246	1.779080436	37.401069374
-1.155062380	3.844534556	37.465901750

-1.425700346	4.893738431	38.576737578
2.667198174	6.586108369	37.440576995
1.600665471	4.020550643	39.205764750
2.775253883	6.412516454	38.399288579
2.887200719	1.763515258	38.369556557
-1.066962424	3.996465960	38.430182484

Ag(111)_Volmer

1.0

8.6679000854	0.0000000000	0.0000000000
-4.3339500427	7.5066216715	0.0000000000
0.0000000000	0.0000000000	60.1641006470

Ag O H

27 4 9

Cartesian

-0.002519736	0.331844687	34.806196468
1.440968624	1.168455363	32.377071249
-0.000043269	2.001790716	30.000227196
2.887282398	0.328193942	34.769801547
4.333350797	1.166338574	32.384831482
2.889314839	2.001790716	30.000227196
5.770983382	0.330567947	34.802033053
7.223097682	1.165162506	32.400606560
5.778585246	2.001790716	30.000227196
-1.454563353	2.831202894	34.801226189
-0.000662987	3.666504140	32.379208540

-1.444679119	4.503973629	30.000227196
1.436965707	2.832180304	34.771440376
2.882721260	3.669018023	32.382339171
1.444678860	4.503973629	30.000227196
4.337232560	2.838959532	34.772024904
5.780318210	3.669968811	32.396019989
4.333949784	4.503973629	30.000227196
-2.891344746	5.333074844	34.804758458
-1.448596983	6.167918817	32.394036898
-2.889314452	7.006155648	30.000227196
-0.001913144	5.343643577	34.782675502
1.446117464	6.169896456	32.395148576
0.000043398	7.006155648	30.000227196
2.890896037	5.345210922	34.803887046
4.333419446	6.171626218	32.409460541
2.889314322	7.006155648	30.000227196
-0.742271288	4.136627283	38.840822198
1.472249217	2.801233170	38.239271416
-0.699986306	6.741452318	37.983911681
5.589881699	2.939197167	38.019926480
-0.753199924	5.065039507	38.481889881
-1.569367442	3.700651290	38.500537393
2.201802719	3.448169273	38.268153542
0.632060515	3.337055298	38.425323373
-1.605986161	7.098171318	38.064095979
-0.512483447	6.763015289	37.015697038

1.371187360	2.746072270	36.438617529
5.539330880	3.007078489	37.037209811
5.620774355	1.979659062	38.199225886

Ag(111)_Heyrovsky

1.0

8.6679000854	0.0000000000	0.0000000000
-4.3339500427	7.5066216715	0.0000000000
0.0000000000	0.0000000000	60.1641006470

Ag H O

27 10 4

Cartesian

-0.010318654	0.319824353	34.814860389
1.444052167	1.176370503	32.437851377
-0.000043269	2.001790716	30.000227196
2.897987633	0.321084203	34.812457729
4.332756523	1.168527623	32.403507682
2.889314839	2.001790716	30.000227196
5.779474993	0.333570199	34.816997680
7.224467636	1.168594626	32.403586575
5.778585246	2.001790716	30.000227196
-1.464862051	2.834351008	34.809345029
0.005816930	3.666320247	32.433938986
-1.444679119	4.503973629	30.000227196
1.442223495	2.835973388	34.892555961
2.882268935	3.666141498	32.435477406

1.444678860	4.503973629	30.000227196
4.350491533	2.834475841	34.810302507
5.777995494	3.672123407	32.395711588
4.333949784	4.503973629	30.000227196
-2.889794401	5.339375994	34.806217985
-1.446851361	6.172134945	32.394675217
-2.889314452	7.006155648	30.000227196
-0.009688167	5.357276307	34.807329663
1.444627712	6.170555519	32.404561984
0.000043398	7.006155648	30.000227196
2.897386158	5.355844532	34.810230785
4.335233136	6.171924654	32.394954929
2.889314322	7.006155648	30.000227196
1.433451085	2.933569846	36.724300987
0.738913082	3.885762949	39.298328127
-0.908838961	5.083636467	39.632997162
0.452817939	5.935450547	39.607848124
1.326015741	2.977737627	37.674499265
2.111915939	2.981562031	39.327389556
-2.762328704	4.847312697	38.393357236
-2.976269066	5.951653759	39.464183395
5.182784608	0.298675479	38.395828031
6.323701444	0.111991112	39.434695225
0.065522478	5.048432713	39.864308780
1.200774024	2.988499650	38.958774878
-2.574141764	5.073342456	39.321884954

1.031135401 7.501699499 39.304636006

Metal(100)

Pt(100)_Rf_sur

1.0

8.3664999008	0.0000000000	0.0000000000
0.0000000000	8.3664999008	0.0000000000
0.0000000000	0.0000000000	43.9440002441

Pt H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999845281
8.365285610	0.000107664	18.896441653
1.396442713	1.399791240	16.959340831
2.788805457	0.000000000	14.999845281
2.787860454	0.001280605	18.908469325
4.180010012	1.399274106	16.959175818
5.577694693	0.000000000	14.999845281
5.577607922	8.365857099	18.898256805
6.971495637	1.398266020	16.952232142
0.000000000	2.788805457	14.999845281
8.362879468	2.789496880	18.917628900
1.396440220	4.180298499	16.959518941
2.788805457	2.788805457	14.999845281
2.787156066	2.790492998	18.930358536
4.180001036	4.180768757	16.959627641

5.577694693	2.788805457	14.999845281
5.578940900	2.789773399	18.913160432
6.971479180	4.180645582	16.952517642
0.000000000	5.577694693	14.999845281
8.365222277	5.579852990	18.896617144
1.396848765	6.972927852	16.950210068
2.788805457	5.577694693	14.999845281
2.787749248	5.580732167	18.908562309
4.180431149	6.972906908	16.950682846
5.577694693	5.577694693	14.999845281
5.577454328	5.580961062	18.898914241
6.971345533	6.972413212	16.946696322
5.761008295	3.695122056	23.662899058
5.011713273	5.086978389	23.704925190
3.550117225	3.379276165	23.460882889
7.117421035	2.676870989	22.095247089
2.697068618	2.927641340	22.226178984
5.203599223	6.811394696	22.201086411
4.249602118	7.224661158	23.350376034
7.941319920	3.444371653	23.161749556
4.969433994	4.155639659	24.051325807
2.705477398	2.908326129	23.192722382
7.184462880	2.837044488	23.057164862
5.096311227	6.773371172	23.170513621

Pt(100)_Rf_top

1.0

8.3664999008	0.0000000000	0.0000000000
0.0000000000	8.3664999008	0.0000000000
0.0000000000	0.0000000000	43.9440002441

Pt H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999845281
8.362714903	8.365043749	18.890945123
1.406526941	1.409176814	16.963581424
2.788805457	0.000000000	14.999845281
2.787908328	0.001079222	18.887322677
4.171177352	1.408249389	16.962668609
5.577694693	0.000000000	14.999845281
5.579782177	8.364061345	18.894671029
6.971710070	1.394306608	16.944399225
0.000000000	2.788805457	14.999845281
8.363328780	2.789419335	18.896779539
1.407792970	4.169041496	16.965632310
2.788805457	2.788805457	14.999845281
2.784578626	2.795145205	19.077816693
4.169822681	4.170201431	16.964322676
5.577694693	2.788805457	14.999845281
5.578811243	2.789828005	18.891927347
6.971744978	4.184651746	16.944752826
0.000000000	5.577694693	14.999845281

8.362866502	5.581836249	18.891108827
1.392665943	6.972230196	16.942341792
2.788805457	5.577694693	14.999845281
2.788093838	5.580749122	18.888899475
4.184672691	6.972375811	16.942662652
5.577694693	5.577694693	14.999845281
5.579375252	5.583245525	18.895272151
6.971239813	6.972268594	16.938394557
2.828876322	2.693831920	20.635713204
5.759501776	3.691887603	23.664756118
5.011077952	5.088226590	23.705365226
3.554169018	3.380770716	23.466922918
7.118563018	2.673388192	22.107693844
2.696099179	2.928617510	22.238822184
5.203893446	6.812692268	22.209051600
4.248878031	7.221953812	23.357042068
7.936550523	3.449209370	23.172354966
4.970037899	4.157002309	24.052750688
2.706258833	2.909170648	23.207678394
7.182638202	2.836736302	23.068642488
5.098297977	6.774200979	23.178009962

Pt(100)_Rf_min

1.0

8.3664999008	0.0000000000	0.0000000000
0.0000000000	8.3664999008	0.0000000000

0.0000000000 0.0000000000 43.9440002441

Pt H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999845281
8.360265874	8.365057213	18.890654384
1.396893272	1.394816261	16.955240370
2.788805457	0.000000000	14.999845281
2.789443272	8.362006774	18.902500017
4.181487109	1.393872006	16.955755055
5.577694693	0.000000000	14.999845281
5.575318472	8.364843777	18.910529378
6.970749109	1.393399255	16.941965927
0.000000000	2.788805457	14.999845281
8.354827245	2.787064308	18.898720415
1.400932599	4.182326142	16.959025210
2.788805457	2.788805457	14.999845281
2.788869538	2.751646149	18.959285715
4.177743002	4.182460287	16.960244478
5.577694693	2.788805457	14.999845281
5.591392497	2.782863159	18.897520791
6.971828757	4.183201578	16.940383890
0.000000000	5.577694693	14.999845281
8.355395743	5.576782603	18.899800863
1.397867324	6.967153610	16.956963847
2.788805457	5.577694693	14.999845281

2.787355539	5.602720563	18.970012921
4.180596462	6.967489722	16.958369083
5.577694693	5.577694693	14.999845281
5.590840955	5.579583701	18.901541365
6.970215519	6.971461228	16.943034588
2.827095777	4.171493516	19.979565985
5.774316130	5.200539808	22.986182740
5.031166868	6.591684770	23.034856569
3.552852497	4.894496513	22.894463884
7.116975214	4.237217344	21.340511988
2.636932275	4.456111925	21.709303405
5.163171552	8.276122718	21.447891439
4.275692176	0.369573014	22.642377816
7.948859995	4.897521021	22.470902294
5.013553411	5.673711473	23.418560780
2.687325364	4.437752938	22.677651478
7.173333789	4.324762510	22.321520286
5.105866478	8.265684800	22.436699912

Pt(100)_Volmer

1.0

8.3664999008	0.0000000000	0.0000000000
0.0000000000	8.3664999008	0.0000000000
0.0000000000	0.0000000000	43.9440002441

Pt O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999845281
8.363818486	8.363645942	18.894719486
1.403609774	1.404882786	16.961420529
2.788805457	0.000000000	14.999845281
2.787735534	0.011326039	18.893739880
4.177357272	1.404161816	16.964258504
5.577694693	0.000000000	14.999845281
5.578477624	8.360740619	18.910825355
6.970376095	1.392669434	16.949195102
0.000000000	2.788805457	14.999845281
0.003526560	2.787253059	18.897622943
1.403498818	4.175788417	16.961533157
2.788805457	2.788805457	14.999845281
2.794357287	2.797373566	19.030546790
4.177381208	4.176971291	16.963711078
5.577694693	2.788805457	14.999845281
5.579419635	2.789332814	18.901025370
6.971154039	4.183799498	16.949277609
0.000000000	5.577694693	14.999845281
8.363045529	5.580488810	18.893928467
1.393657074	6.973840939	16.945628971
2.788805457	5.577694693	14.999845281
2.788483308	5.579599161	18.892067478
4.184668701	6.974603425	16.948451231
5.577694693	5.577694693	14.999845281

5.578617255	5.586872940	18.908474564
6.969420620	6.972313974	16.945056661
4.917033959	4.139169930	22.979176202
2.839850074	2.997215493	22.074921581
7.143514584	2.853919646	22.130164531
5.115221757	6.735127728	22.180360155
5.742411935	3.686042050	22.630384194
4.965349787	5.083500579	22.645926922
2.873525837	2.066614689	22.376564172
3.731142873	3.463764159	22.399967318
7.084329478	2.746841096	21.140994599
2.848469548	2.927441368	20.750134552
5.199917452	6.749352640	21.188918009
4.282936034	7.212545673	22.361464100
7.905549442	3.452389965	22.253236007

Pt(100)_Heyrovsky

1.0

8.3664999008	0.0000000000	0.0000000000
0.0000000000	8.3664999008	0.0000000000
0.0000000000	0.0000000000	43.9440002441

Pt H O

27 10 4

Cartesian

0.000000000	0.000000000	14.999845281
0.000421779	0.001819618	18.890053262

1.404791153	1.407436163	16.963565708
2.788805457	0.000000000	14.999845281
2.788344425	8.352574698	18.888805182
4.172924984	1.406649617	16.963612855
5.577694693	0.000000000	14.999845281
5.576858403	0.001153510	18.893357467
6.971528051	1.393417706	16.941694833
0.000000000	2.788805457	14.999845281
8.348937309	2.789997308	18.895125472
1.404227392	4.173277303	16.963124362
2.788805457	2.788805457	14.999845281
2.784378156	2.785857996	19.032105253
4.173238405	4.173743321	16.963603688
5.577694693	2.788805457	14.999845281
5.593391216	2.790084078	18.891696852
6.971537027	4.186077977	16.942191184
0.000000000	5.577694693	14.999845281
0.000372009	5.578821715	18.890651765
1.391975019	6.972956277	16.939748718
2.788805457	5.577694693	14.999845281
2.788191579	5.595501140	18.887470665
4.186090943	6.972847066	16.940728323
5.577694693	5.577694693	14.999845281
5.576594600	5.579299951	18.894174678
6.971347029	6.972519930	16.944142537
2.823303298	2.844182626	20.818042966

5.778427266	3.710739289	23.734646007
5.016860672	5.105941779	23.754830075
2.867185841	2.020155206	23.523674565
3.625720946	3.416926426	23.575263639
7.105954834	2.671225158	22.223784975
2.804271090	2.902405524	21.659238745
5.213691056	6.811717842	22.273014089
4.273686975	7.231451715	23.432068338
7.953794456	3.461441048	23.253808916
4.968553322	4.169152702	24.092786177
2.754151030	2.964788929	23.294315873
7.192774916	2.855985686	23.179261972
5.113150729	6.772311971	23.243507341

Ir(100)_Rf_sur

1.0

8.2730998993	0.0000000000	0.0000000000
0.0000000000	8.2730998993	0.0000000000
0.0000000000	0.0000000000	43.9000015259

Ir H O

27 8 4

Cartesian

0.000000000	0.000000000	15.000191691
0.001270117	0.000914533	18.672316610
1.378100859	1.378408686	16.835456074
2.757672434	0.000000000	15.000191691

2.757333417	0.001771657	18.669261678
4.139895243	1.380643114	16.837320433
5.515427712	0.000000000	15.000191691
5.513873906	8.268339365	18.676407733
6.891972546	1.378518404	16.838168226
0.000000000	2.757672434	15.000191691
8.271245786	2.756673876	18.675253793
1.378238068	4.137784710	16.836681972
2.757672434	2.757672434	15.000191691
2.756013841	2.757198304	18.673365884
4.139192061	4.134642334	16.837736480
5.515427712	2.757672434	15.000191691
5.518593511	2.757273011	18.676691639
6.892822183	4.136611589	16.838677163
0.000000000	5.515427712	15.000191691
0.000656024	5.515141705	18.672315302
1.377683807	6.893777840	16.836921395
2.757672434	5.515427712	15.000191691
2.758328277	5.514565253	18.670286094
4.136492502	6.894385358	16.836171726
5.515427712	5.515427712	15.000191691
5.513372408	5.520724262	18.676299142
6.895485498	6.894150142	16.837221001
5.770628625	3.491484038	23.244153634
5.039762891	4.889942171	23.284523218
3.568396692	3.192306127	23.125494062

7.110301758	2.567480375	21.589891675
2.700513481	2.720843387	21.911540021
5.138531889	6.582586164	21.700993070
4.271282824	7.005934916	22.917740379
7.922926482	3.212863113	22.745120374
5.008318415	3.971874382	23.665836281
2.717524969	2.720398844	22.877462378
7.162728777	2.626682057	22.569151065
5.106099211	6.559622776	22.680913164

Ir(100)_Rf_top

1.0

8.2730998993	0.0000000000	0.0000000000
0.0000000000	8.2730998993	0.0000000000
0.0000000000	0.0000000000	43.9000015259

Ir H O

27 9 4

Cartesian

0.000000000	0.000000000	15.000191691
8.268804373	8.268186993	18.663499828
1.390919018	1.392337957	16.847993724
2.757672434	0.000000000	15.000191691
2.757676379	8.252789964	18.666405611
4.126432705	1.392687699	16.848013349
5.515427712	0.000000000	15.000191691
5.519535854	8.263154752	18.667030989

6.892761530	1.376870537	16.829966355
0.000000000	2.757672434	15.000191691
8.250202589	2.756595717	18.673771464
1.391170384	4.123511738	16.849207847
2.757672434	2.757672434	15.000191691
2.758589628	2.756999825	18.723536108
4.125850336	4.122435760	16.848654427
5.515427712	2.757672434	15.000191691
5.539645091	2.757176853	18.673346260
6.893483944	4.138467181	16.830439968
0.000000000	5.515427712	15.000191691
8.268364021	5.520918549	18.663354604
1.375771136	6.893870053	16.828510193
2.757672434	5.515427712	15.000191691
2.758577054	5.536237665	18.667292654
4.139194033	6.894394728	16.827678100
5.515427712	5.515427712	15.000191691
5.519037315	5.525810745	18.667219388
6.895542700	6.893986921	16.820641944
2.802478112	2.756472438	20.329356137
5.768760705	3.488999477	23.249266556
5.038971441	4.892537436	23.288411551
3.575033776	3.194620070	23.136502283
7.109935373	2.557735186	21.618507293
2.700523343	2.722289201	21.926312285
5.146814252	6.586251489	21.727600415

4.267278236	6.994921681	22.938984911
7.911511358	3.225671779	22.766877769
5.007273011	3.973491306	23.668049961
2.722654599	2.720088674	22.896605745
7.161319947	2.625163016	22.596801143
5.109868090	6.561094725	22.706762990

Ir(100)_Rf_min

1.0

8.2730998993	0.0000000000	0.0000000000
0.0000000000	8.2730998993	0.0000000000
0.0000000000	0.0000000000	43.9000015259

Ir H O

27 9 4

Cartesian

0.000000000	0.000000000	15.000191691
8.271389776	8.272692093	18.661494171
1.381484122	1.382696076	16.835576440
2.757672434	0.000000000	15.000191691
2.760934884	8.272827700	18.666553452
4.133390807	1.387507154	16.833379767
5.515427712	0.000000000	15.000191691
5.514221059	8.271435636	18.659470196
6.897255289	1.379180905	16.824654568
0.000000000	2.757672434	15.000191691
8.254490225	2.756136380	18.667912798

1.379473445	4.135866985	16.834893496
2.757672434	2.757672434	15.000191691
2.758508018	2.731269321	18.692886049
4.140011125	4.136772345	16.836302559
5.515427712	2.757672434	15.000191691
5.536110442	2.751255280	18.667737483
6.890867475	4.137465171	16.825728700
0.000000000	5.515427712	15.000191691
8.257528801	5.518670437	18.665897982
1.380674057	6.890618945	16.833956737
2.757672434	5.515427712	15.000191691
2.756936953	5.542705364	18.691915274
4.134443362	6.885823399	16.833212302
5.515427712	5.515427712	15.000191691
5.534367773	5.523985726	18.670821198
6.895928316	6.894402617	16.824928007
2.804343320	4.135866985	19.792647129
5.784924527	4.869143066	22.736208085
5.052313165	6.267249855	22.778215687
3.587135809	4.569968607	22.648265297
7.121640448	3.939378091	21.095565757
2.695367578	4.086132867	21.462124873
5.153709481	7.949255874	21.208451704
4.280261465	0.109254707	22.421726726
7.937366867	4.589069916	22.247319554
5.030150104	5.352356987	23.169806928

2.728229266	4.098818009	22.431651657
7.174315012	4.003923417	22.080427383
5.120404975	7.939159340	22.198767724

Ir(100)_Volmer

1.0

8.2730998993	0.0000000000	0.0000000000
0.0000000000	8.2730998993	0.0000000000
0.0000000000	0.0000000000	43.9000015259

Ir O H

27 4 9

Cartesian

0.000000000	0.000000000	15.000191691
8.269768906	8.267445348	18.661513795
1.384057814	1.381152749	16.842837627
2.757672434	0.000000000	15.000191691
2.756802086	8.264626701	18.669819023
4.133935453	1.381885025	16.844204824
5.515427712	0.000000000	15.000191691
5.519332691	8.263521630	18.665238588
6.893103752	1.380962406	16.830701632
0.000000000	2.757672434	15.000191691
8.260819359	2.757039767	18.666934173
1.384213268	4.134166724	16.843092750
2.757672434	2.757672434	15.000191691
2.757740977	2.762775683	18.690480044

4.132655079	4.132185634	16.842213557
5.515427712	2.757672434	15.000191691
5.528454829	2.757212111	18.668863948
6.895613708	4.132695515	16.829474426
0.000000000	5.515427712	15.000191691
8.267894575	5.521364325	18.660499846
1.381596429	6.894750264	16.831139920
2.757672434	5.515427712	15.000191691
2.757512172	5.525398994	18.669570442
4.131925762	6.895340029	16.830103729
5.515427712	5.515427712	15.000191691
5.520809571	5.525403432	18.657554813
6.895807009	6.895917960	16.820873517
4.804036082	4.023364483	22.721536562
2.711356098	2.876560778	21.816599019
7.046672147	2.723822296	21.909632488
4.995017126	6.632491393	21.937347981
5.633340427	3.569201949	22.389882169
4.860305456	4.968325788	22.396180431
2.757612521	1.936996619	22.087377189
3.598415325	3.334188678	22.144001365
6.980593234	2.616363129	20.921671447
2.742890320	2.836498375	20.461397227
5.088554173	6.654698342	20.948328508
4.150286166	7.091451444	22.110118442
7.799121533	3.335488037	22.029889521

Ir(100)_Heyrovsky

1.0

8.2730998993	0.0000000000	0.0000000000
0.0000000000	8.2730998993	0.0000000000
0.0000000000	0.0000000000	43.9000015259

Ir H O

27 10 4

Cartesian

0.000000000	0.000000000	15.000191691
0.002745501	0.001586902	18.663977366
1.397453411	1.399415639	16.848599477
2.757672434	0.000000000	15.000191691
2.757123350	8.241237262	18.658645954
4.119550543	1.400452661	16.850050406
5.515427712	0.000000000	15.000191691
5.512125812	8.269946921	18.669062813
6.892303426	1.363993080	16.824051431
0.000000000	2.757672434	15.000191691
8.236625649	2.757134199	18.666802033
1.397359226	4.116791811	16.849303354
2.757672434	2.757672434	15.000191691
2.757927868	2.757527705	18.750762289
4.119454139	4.115216308	16.850322537
5.515427712	2.757672434	15.000191691
5.550627753	2.757368675	18.668459677

6.892647620	4.151745294	16.824555135
0.000000000	5.515427712	15.000191691
0.002545301	5.514644645	18.663749718
1.362378621	6.894149649	16.821803734
2.757672434	5.515427712	15.000191691
2.757689693	5.548694741	18.659322356
4.152242354	6.894451929	16.821430863
5.515427712	5.515427712	15.000191691
5.511553306	5.519650750	18.669235512
6.894569783	6.894157539	16.829053146
2.698347473	2.776159569	20.566293251
5.721725899	3.568429978	23.293733804
4.956614795	4.954264115	23.326473254
2.812480214	1.844933740	23.261604033
3.571605886	3.244721312	23.283903073
7.058816588	2.613860323	21.646653224
2.721769704	2.773626190	21.410495870
5.084448002	6.652041930	21.731552856
4.223681430	7.120099956	22.937103544
7.900433033	3.246182412	22.787562340
4.946409284	4.035452708	23.710533793
2.698818398	2.787342435	23.021265282
7.112145515	2.693573871	22.624985015
5.033173393	6.623548749	22.710941770

Rh(100)_Rf_sur

1.0

8.0700998306	0.0000000000	0.0000000000
0.0000000000	8.0700998306	0.0000000000
0.0000000000	0.0000000000	43.8042984009

Rh H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999905706
8.069786690	0.000005189	18.717768880
1.345144148	1.344711594	16.860063129
2.690006420	0.000000000	14.999905706
2.690266650	0.000379998	18.718485583
4.036002807	1.345767303	16.860368609
5.380093651	0.000000000	14.999905706
5.379127772	8.065036181	18.720447704
6.724259052	1.345636106	16.860204120
0.000000000	2.690006420	14.999905706
8.066396974	2.690025901	18.720234913
1.345370225	4.035455411	16.860239368
2.690006420	2.690006420	14.999905706
2.689632190	2.690169725	18.718067833
4.035567969	4.034138632	16.859821617
5.380093651	2.690006420	14.999905706
5.383583418	2.690103585	18.723091281
6.724626067	4.034046998	16.859719791
0.000000000	5.380093651	14.999905706

8.069295573	5.379746358	18.717831543
1.344954868	6.724854069	16.860360776
2.690006420	5.380093651	14.999905706
2.690691627	5.379400989	18.719584789
4.034344025	6.724966145	16.859629713
5.380093651	5.380093651	14.999905706
5.379183089	5.384690715	18.719238839
6.725364907	6.725072931	16.858577505
5.686618812	3.549179112	23.215543225
4.961224449	4.948234146	23.243490723
3.491713641	3.274172728	23.059696238
7.031988676	2.680191781	21.547757224
2.674838561	2.808115671	21.808616204
5.005101715	6.598840050	21.619256501
4.254688778	7.088916853	22.889700568
7.841894565	3.256561069	22.743038867
4.923082330	4.033009448	23.630891504
2.641813484	2.818145084	22.774764394
7.073662891	2.692954323	22.529356955
5.047575859	6.597540828	22.598763564

Rh(100)_Rf_top

1.0

8.0700998306	0.0000000000	0.0000000000
0.0000000000	8.0700998306	0.0000000000
0.0000000000	0.0000000000	43.8042984009

Rh H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999905706
8.062950979	8.064584027	18.710618822
1.343342264	1.344915665	16.855517483
2.690006420	0.000000000	14.999905706
2.690170687	8.068991090	18.711855102
4.037391979	1.346578776	16.856141498
5.380093651	0.000000000	14.999905706
5.385449758	8.060026405	18.713189292
6.724289837	1.346597055	16.857666287
0.000000000	2.690006420	14.999905706
8.064072226	2.689999686	18.713873358
1.346488947	4.036488632	16.859469140
2.690006420	2.690006420	14.999905706
2.688496513	2.686346614	18.727762252
4.034253354	4.034690597	16.859662350
5.380093651	2.690006420	14.999905706
5.385235706	2.690203637	18.716387693
6.724705916	4.031504591	16.858521369
0.000000000	5.380093651	14.999905706
8.064176607	5.385321808	18.711332914
1.346680992	6.725379818	16.858689775
2.690006420	5.380093651	14.999905706
2.690689703	5.382388576	18.714734968

4.032162861	6.725535667	16.858162365
5.380093651	5.380093651	14.999905706
5.383846533	5.389727909	18.712734989
6.725119108	6.724064722	16.847924871
2.647886304	2.426220202	20.291828675
5.684854928	3.548358018	23.216645042
4.959290286	4.948755567	23.246341869
3.500289665	3.272989430	23.072009429
7.028313237	2.678806216	21.567531175
2.682278186	2.809680655	21.819834106
5.010205289	6.595897679	21.637638821
4.255476200	7.076587465	22.908551553
7.821903082	3.271446092	22.764738386
4.926171412	4.034940484	23.637538956
2.647349009	2.822352766	22.792866039
7.071114472	2.685815814	22.548544750
5.054742989	6.598420605	22.617865198

Rh(100)_Rf_min

1.0

8.0700998306	0.0000000000	0.0000000000
0.0000000000	8.0700998306	0.0000000000
0.0000000000	0.0000000000	43.8042984009

Rh H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999905706
8.064567191	8.069590916	18.697101987
1.348870574	1.345009944	16.851513607
2.690006420	0.000000000	14.999905706
2.686274221	8.070035856	18.700776885
4.031886517	1.344002097	16.845482337
5.380093651	0.000000000	14.999905706
5.384001420	8.069507701	18.689378828
6.719780318	1.346044729	16.849751223
0.000000000	2.690006420	14.999905706
8.069058913	2.687979421	18.688984576
1.341209081	4.035639159	16.846197734
2.690006420	2.690006420	14.999905706
2.685570255	2.686115246	18.709601861
4.036120175	4.035552576	16.820952559
5.380093651	2.690006420	14.999905706
5.382823895	2.685448558	18.711609674
6.727364488	4.035414044	16.846426191
0.000000000	5.380093651	14.999905706
8.069930032	5.378707845	18.702007943
1.346620745	6.722899703	16.854614098
2.690006420	5.380093651	14.999905706
2.686897136	5.384106763	18.710477831
4.033282424	6.727405374	16.845793039
5.380093651	5.380093651	14.999905706
5.382812350	5.384888413	18.712896867

6.722901627	6.720821235	16.851576270
4.029024716	4.024461563	19.254213845
7.066873839	4.789097405	22.380141754
6.303403738	6.172251994	22.405773349
4.844138077	4.493569700	22.275774664
0.312000981	3.870417092	20.788965944
3.955220353	3.989994402	21.093511166
6.444945415	7.800524832	20.851101086
5.595488514	0.266169830	22.046333121
1.220802139	4.448386959	21.910932401
6.284594110	5.252082938	22.786458793
3.973898423	4.036995623	22.063019636
0.398510073	3.936785437	21.780966353
6.399768927	7.820601454	21.846273787

Rh(100)_Volmer

1.0

8.0700998306	0.0000000000	0.0000000000
0.0000000000	8.0700998306	0.0000000000
0.0000000000	0.0000000000	43.8042984009

Rh O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999905706
8.068941064	8.069235927	18.706951757
1.347047405	1.343327112	16.856940445

2.690006420	0.000000000	14.999905706
2.691832355	0.005424422	18.712520892
4.036996104	1.346522618	16.858035735
5.380093651	0.000000000	14.999905706
5.384558917	8.062837941	18.707622769
6.725909416	1.350639989	16.854228985
0.000000000	2.690006420	14.999905706
8.069401396	2.690432840	18.703729858
1.347428249	4.038042312	16.856768123
2.690006420	2.690006420	14.999905706
2.701453625	2.707344381	18.718909861
4.038327554	4.036620431	16.856060559
5.380093651	2.690006420	14.999905706
5.388761068	2.691231807	18.715088751
6.726077291	4.033510906	16.854842555
0.000000000	5.380093651	14.999905706
8.067688019	5.385335276	18.705592763
1.349401976	6.727144183	16.857328170
2.690006420	5.380093651	14.999905706
2.691411707	5.383977370	18.711986954
4.032510394	6.727066258	16.856187189
5.380093651	5.380093651	14.999905706
5.386799006	5.392892991	18.707719374
6.726542914	6.726709345	16.846393555
4.910353219	4.141075818	22.701921789
2.814699330	2.990768295	21.799671125

7.165571953	2.850129002	21.912120379
5.120034581	6.751209385	21.936613604
5.747866507	3.691966379	22.384045109
4.972559097	5.088555007	22.384998102
2.860487670	2.057416049	22.094457960
3.704718819	3.452281920	22.107434330
7.062107939	2.698574267	20.930179920
2.808154634	2.911855067	20.441090873
5.207556782	6.776460771	20.943805109
4.272829794	7.204982510	22.113859853
7.925308894	3.461631898	21.971764684

Rh(100)_Heyrovsky

1.0

8.0700998306	0.0000000000	0.0000000000
0.0000000000	8.0700998306	0.0000000000
0.0000000000	0.0000000000	43.8042984009

Rh H O

27 10 4

Cartesian

0.0000000000	0.0000000000	14.999905706
8.066644697	8.068472074	18.706020957
1.353026548	1.354665608	16.860627092
2.690006420	0.0000000000	14.999905706
2.690342650	8.057396213	18.700770358
4.027993900	1.355188712	16.860586623

5.380093651	0.000000000	14.999905706
5.382269765	8.064211240	18.709925618
6.724316293	1.342073465	16.850919619
0.000000000	2.690006420	14.999905706
8.052426843	2.690620917	18.706075787
1.352909541	4.027976102	16.860120570
2.690006420	2.690006420	14.999905706
2.689551620	2.697800073	18.791768132
4.028158407	4.027424618	16.860026576
5.380093651	2.690006420	14.999905706
5.397999931	2.690843387	18.706956979
6.724417788	4.038825405	16.850890898
0.000000000	5.380093651	14.999905706
8.066656722	5.384046155	18.705523573
1.340898705	6.726353394	16.849866104
2.690006420	5.380093651	14.999905706
2.690259675	5.397719018	18.701339542
4.038785000	6.726276431	16.850200305
5.380093651	5.380093651	14.999905706
5.382303436	5.388026076	18.709808125
6.725063310	6.725463996	16.843791753
2.693516630	2.590245743	20.549568888
5.690312530	3.566213311	23.353646267
4.929210948	4.958741448	23.372118665
2.754208993	1.922709480	23.172765590
3.571690875	3.299038099	23.197611292

7.035820445	2.581438110	21.780997684
2.713426340	2.762222951	21.390579963
5.098031492	6.654682094	21.833014130
4.221270711	7.095816538	23.037223880
7.874089409	3.303886975	22.869486674
4.886495816	4.025974357	23.722780914
2.691644278	2.860767380	22.896113036
7.102004802	2.717253780	22.748827320
5.038702567	6.611784657	22.808949427

Pd(100)_Rf_sur

1.0

8.2524003983	0.0000000000	0.0000000000
0.0000000000	8.2524003983	0.0000000000
0.0000000000	0.0000000000	43.8902015686

Pd H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999915706
8.251368431	8.252280871	18.951102665
1.378426654	1.379015927	16.982075496
2.750772669	0.000000000	14.999915706
2.751202328	0.000311677	18.958022143
4.123534202	1.378935997	16.981868827
5.501627975	0.000000000	14.999915706
5.502376126	8.251480580	18.952026134

6.877103955	1.377791143	16.976797595
0.000000000	2.750772669	14.999915706
8.252296611	2.751016397	18.962734975
1.378637917	4.122883197	16.982219379
2.750772669	2.750772669	14.999915706
2.750941877	2.751176504	18.983276277
4.123279161	4.122834501	16.981764185
5.501627975	2.750772669	14.999915706
5.502656007	2.751215363	18.961415173
6.877270211	4.123861057	16.976487592
0.000000000	5.501627975	14.999915706
8.251381712	5.501949173	18.951157602
1.377281431	6.876798005	16.976539913
2.750772669	5.501627975	14.999915706
2.751294801	5.501143964	18.960368749
4.124353922	6.876836863	16.976487592
5.501627975	5.501627975	14.999915706
5.502273323	5.502366781	18.951377351
6.876988855	6.877056242	16.973933009
5.614525084	3.572947009	23.650361100
4.862731594	4.967569227	23.689301152
3.456302009	3.292311212	23.356491247
6.982382805	2.541900400	22.179470972
2.688604764	2.848035083	22.060945148
5.087515980	6.683142824	22.264976889
4.128178546	7.069437450	23.422026163

7.765691629	3.370349179	23.235406915
4.805442168	4.027090033	24.012421171
2.620440086	2.835097372	23.024063286
7.035436149	2.729819506	23.135128108
4.980818052	6.632592665	23.232134225

Pd(100)_Rf_top

1.0

8.2524003983	0.0000000000	0.0000000000
0.0000000000	8.2524003983	0.0000000000
0.0000000000	0.0000000000	43.8902015686

Pd H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999915706
8.244056614	8.245387645	18.947480730
1.380570519	1.381765422	16.976794979
2.750772669	0.000000000	14.999915706
2.751096819	0.005713726	18.947342079
4.121100373	1.381591418	16.976712573
5.501627975	0.000000000	14.999915706
5.509256071	8.244386175	18.949395686
6.877008530	1.378604715	16.973425494
0.000000000	2.750772669	14.999915706
0.003765110	2.751073455	18.952803104
1.380880773	4.120427233	16.977061817

2.750772669	2.750772669	14.999915706
2.749151674	2.752372514	19.025231337
4.120767123	4.120504459	16.976734810
5.501627975	2.750772669	14.999915706
5.497708172	2.751281029	18.950490507
6.877132976	4.123354665	16.973259374
0.000000000	5.501627975	14.999915706
8.244135807	5.509431181	18.947280601
1.377749825	6.877118711	16.972669453
2.750772669	5.501627975	14.999915706
2.751146253	5.497580283	18.948298249
4.123856384	6.877120187	16.972882661
5.501627975	5.501627975	14.999915706
5.509142447	5.510107518	18.948690658
6.876803415	6.877108874	16.967906916
2.764594537	2.735627887	20.580664673
5.628564855	3.572386510	23.697047305
4.900849451	4.974701507	23.735869634
3.405168725	3.276616015	23.429565647
7.004660606	2.526168311	22.148583153
2.598343790	2.813081499	22.168700654
5.083122496	6.717028041	22.237063530
4.124469760	7.103940471	23.389652422
7.814574802	3.342268900	23.189272700
4.835391842	4.041221048	24.069341402
2.563108358	2.815269142	23.141982185

7.068232833	2.721292988	23.104470503
4.980165817	6.675615563	23.208466731

Pd(100)_Rf_min

1.0

8.2524003983	0.0000000000	0.0000000000
0.0000000000	8.2524003983	0.0000000000
0.0000000000	0.0000000000	43.8902015686

Pd H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999915706
8.243859370	0.002931677	18.964304611
1.372353886	1.369564058	16.974560864
2.750772669	0.000000000	14.999915706
2.748142334	8.252012304	18.945412735
4.123354419	1.370086190	16.965026634
5.501627975	0.000000000	14.999915706
5.502629937	0.001219840	18.934940647
6.877565340	1.372724273	16.973140343
0.000000000	2.750772669	14.999915706
8.252008861	2.750045669	18.940159686
1.368164778	4.127650757	16.966597578
2.750772669	2.750772669	14.999915706
2.747849172	2.751246105	18.953225597
4.127825867	4.126663060	16.946125601

5.501627975	2.750772669	14.999915706
5.500993448	2.749019112	18.963964523
6.882061136	4.127254793	16.969177013
0.000000000	5.501627975	14.999915706
0.000125281	5.503092306	18.952593819
1.371473172	6.879909646	16.979097112
2.750772669	5.501627975	14.999915706
2.750887524	5.499180865	18.958973081
4.123976403	6.882438409	16.966745385
5.501627975	5.501627975	14.999915706
5.501958519	5.504567950	18.967467427
6.880167392	6.877737990	16.975728935
4.146676238	4.128571067	19.234671783
7.020874492	5.010694436	22.521690845
6.268876379	6.401271175	22.560207094
4.804721562	4.713185385	22.328570689
0.117497592	3.961598485	21.000221815
3.915184557	4.213253860	21.140647985
6.478033201	8.125989339	21.081893896
5.511137518	0.288781876	22.230361185
0.981597650	4.739861097	22.031286877
6.232872136	5.473015234	22.916221450
3.940534156	4.251183818	22.111343541
0.205970477	4.147978740	21.976446414
6.367581234	8.100462662	22.071725930

Pd(100)_Volmer

1.0

8.2524003983	0.0000000000	0.0000000000
0.0000000000	8.2524003983	0.0000000000
0.0000000000	0.0000000000	43.8902015686

Pd O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999915706
8.246327631	8.246336976	18.948711586
1.384283977	1.383852966	16.984751725
2.750772669	0.000000000	14.999915706
2.751980484	0.008856695	18.953767122
4.121263677	1.383732209	16.988317415
5.501627975	0.000000000	14.999915706
5.505912262	8.240325694	18.969214955
6.874519610	1.376681089	16.978457485
0.000000000	2.750772669	14.999915706
0.004437485	2.748290390	18.959399499
1.384567670	4.118299600	16.985318102
2.750772669	2.750772669	14.999915706
2.750222008	2.754640579	19.069173295
4.120456500	4.117883469	16.986650985
5.501627975	2.750772669	14.999915706
5.499863104	2.749493532	18.965195379
6.875775875	4.121410504	16.977043505

0.000000000	5.501627975	14.999915706
8.245454049	5.504935877	18.946603042
1.378012121	6.876893922	16.975455556
2.750772669	5.501627975	14.999915706
2.752674037	5.496966907	18.957636274
4.125582888	6.877666175	16.978083388
5.501627975	5.501627975	14.999915706
5.506063761	5.510544801	18.960782086
6.873856554	6.877126090	16.973981407
4.820862158	4.074545029	23.086231333
2.654789394	2.901916509	22.205940266
7.032407635	2.753666162	22.163601953
4.987497801	6.671911696	22.203355599
5.627588470	3.612462301	22.720676207
4.869541200	5.008052049	22.736281004
2.742870595	1.955305276	22.433296798
3.531455830	3.348658685	22.503326104
6.978641555	2.668457302	21.175159047
2.709344697	2.860835312	20.673397455
5.052647984	6.684969180	21.213711921
4.151705233	7.136045569	22.403099618
7.796649660	3.343261517	22.313996619

Pd(100)_Heyrovsky

1.0

8.2524003983	0.0000000000	0.0000000000
--------------	--------------	--------------

0.0000000000	8.2524003983	0.0000000000
0.0000000000	0.0000000000	43.8902015686

Pd H O

27 10 4

Cartesian

0.000000000	0.000000000	14.999915706
8.247345333	8.248732931	18.949100071
1.387505431	1.389235378	16.994011269
2.750772669	0.000000000	14.999915706
2.750777834	8.240533268	18.944218503
4.114396521	1.388941971	16.994036122
5.501627975	0.000000000	14.999915706
5.505609263	8.248005930	18.951999973
6.876838339	1.374468730	16.970676015
0.000000000	2.750772669	14.999915706
8.237689701	2.751447777	18.949699149
1.387537404	4.114318558	16.993682953
2.750772669	2.750772669	14.999915706
2.749928847	2.755833883	19.110225815
4.114348563	4.114549005	16.993611012
5.501627975	2.750772669	14.999915706
5.516793662	2.751620673	18.947891451
6.876878673	4.127702405	16.970560908
0.000000000	5.501627975	14.999915706
8.247443709	5.506527605	18.948850237
1.373428278	6.877757665	16.969400686

2.750772669	5.501627975	14.999915706
2.750769718	5.518495572	18.945376110
4.128188876	6.877670110	16.969929130
5.501627975	5.501627975	14.999915706
5.505492195	5.507020471	18.951901871
6.876337112	6.877162489	16.961061995
2.764751693	2.735007625	20.824450060
5.629395151	3.581154296	23.727801705
4.854042017	4.974698064	23.753028370
2.700887534	1.956010634	23.409144684
3.555310848	3.330353811	23.468615573
6.988545587	2.538802777	22.253447913
2.742662529	2.819683531	21.728866431
5.099418034	6.691026699	22.306954186
4.153916732	7.116501646	23.459870085
7.819055349	3.354090777	23.279911326
4.796214965	4.024153255	24.056023041
2.682479119	2.885732381	23.108041424
7.054378993	2.752660264	23.203647949
4.982177612	6.634184885	23.273154043

Ni(100)_Rf_sur

1.0

7.4579000473	0.0000000000	0.0000000000
0.0000000000	7.4579000473	0.0000000000
0.0000000000	0.0000000000	43.5157012939

Ni H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999862612
7.456211740	7.457137686	18.411164877
1.245449383	1.245404042	16.708492652
2.485941863	0.000000000	14.999862612
2.486265033	0.003684260	18.421397173
3.726564255	1.246213300	16.707907765
4.971958406	0.000000000	14.999862612
4.973061274	7.456125502	18.409172887
6.214728079	1.246116950	16.706653692
0.000000000	2.485941863	14.999862612
0.002950960	2.486101448	18.420910847
1.245977702	3.726860087	16.708172326
2.485941863	2.485941863	14.999862612
2.485765386	2.486342158	18.433871756
3.726712060	3.726533361	16.708086732
4.971958406	2.485941863	14.999862612
4.969296588	2.485833843	18.421320658
6.214449806	3.725542736	16.706156991
0.000000000	4.971958406	14.999862612
7.455863232	4.972737215	18.409963977
1.245858236	6.215001018	16.707331955
2.485941863	4.971958406	14.999862612
2.486251920	4.969300589	18.421089815

3.725455164	6.214688072	16.706415068
4.971958406	4.971958406	14.999862612
4.972461165	4.972630529	18.408938153
6.214967678	6.214667179	16.699702475
5.447727363	3.094863316	23.322655327
4.663824899	4.461709386	23.319994151
3.136392443	2.884775905	22.921105791
6.793606944	1.984615803	21.814062135
2.438528997	2.504272316	21.564233299
4.929383089	6.170456897	21.810599495
3.982428678	6.652057139	22.939080395
0.470181883	2.444827923	22.777731740
4.598497879	3.514076629	23.618110606
2.287967327	2.517065093	22.520728625
6.956197029	2.249317615	22.738446985
4.797952462	6.141670316	22.776336309

Ni(100)_Rf_top

1.0

7.4579000473	0.0000000000	0.0000000000
0.0000000000	7.4579000473	0.0000000000
0.0000000000	0.0000000000	43.5157012939

Ni H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999862612
-------------	-------------	--------------

7.452961814	7.453485465	18.404812813
1.245626305	1.245717432	16.700018911
2.485941863	0.000000000	14.999862612
2.486100559	0.005272041	18.420100304
3.726468682	1.246317653	16.699628553
4.971958406	0.000000000	14.999862612
4.976621479	7.452630642	18.403351242
6.214689405	1.248703310	16.707389017
0.000000000	2.485941863	14.999862612
0.004500495	2.486062330	18.419257340
1.246220746	3.726488908	16.699817896
2.485941863	2.485941863	14.999862612
2.485750495	2.486473960	18.455026282
3.726573368	3.726486908	16.699697287
4.971958406	2.485941863	14.999862612
4.967317560	2.485860293	18.420131429
6.214493814	3.722713998	16.706896207
0.000000000	4.971958406	14.999862612
7.452633309	4.976273860	18.403759755
1.248603292	6.215034357	16.707687297
2.485941863	4.971958406	14.999862612
2.486087890	4.967768754	18.419416854
3.722821795	6.214806316	16.707034972
4.971958406	4.971958406	14.999862612
4.975934242	4.976000477	18.403037399
6.214801870	6.214690739	16.695460416

2.498267221	2.483478525	19.940916486
5.447217937	3.094946442	23.324935222
4.663148331	4.461105276	23.323700603
3.136091943	2.885144639	22.924646243
6.795358819	1.987015574	21.813413701
2.436643098	2.502032797	21.563324194
4.928377573	6.171090346	21.810625432
3.983234158	6.652591903	22.940963448
0.468832859	2.444186918	22.782553499
4.602042080	3.515746489	23.628820150
2.287957325	2.516567224	22.527519030
6.955586251	2.245922551	22.740558288
4.798378762	6.144024967	22.777550178

Ni(100)_Rf_min

1.0

7.4579000473	0.0000000000	0.0000000000
0.0000000000	7.4579000473	0.0000000000
0.0000000000	0.0000000000	43.5157012939

Ni H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999862612
7.450950336	0.002367616	18.408398656
1.247725465	1.246225525	16.708228091
2.485941863	0.000000000	14.999862612

2.487262326	0.000366276	18.409417995
3.729816848	1.239260033	16.701498638
4.971958406	0.000000000	14.999862612
4.978894782	7.457801807	18.416970960
6.207568107	1.248531279	16.708123045
0.000000000	2.485941863	14.999862612
0.001188378	2.483407623	18.413235977
1.235987992	3.730260485	16.699895708
2.485941863	2.485941863	14.999862612
2.477441202	2.483635887	18.427858174
3.731349128	3.728068307	16.682764069
4.971958406	2.485941863	14.999862612
4.976519682	2.481388366	18.436791008
6.219254238	3.729504347	16.701576450
0.000000000	4.971958406	14.999862612
0.000822456	4.965751497	18.429538917
1.245357255	6.208564289	16.714043252
2.485941863	4.971958406	14.999862612
2.484223550	4.973212857	18.427811487
3.729887083	6.219577408	16.700681611
4.971958406	4.971958406	14.999862612
4.975724871	4.976757948	18.435220500
6.212148498	6.206596374	16.712890335
3.737622716	3.725401377	18.912136278
6.708792371	4.334643555	22.396008737
5.924978812	5.701578975	22.390320670

4.409128245	4.134948483	22.058573809
0.600994175	3.263850790	20.880163454
3.666069894	3.741799477	20.730211684
6.175263107	7.406328423	20.870369500
5.250869253	0.435137022	22.021319951
1.731984525	3.690756616	21.864173152
5.868559638	4.759843737	22.707900534
3.547057753	3.757877519	21.696066513
0.762780613	3.469672979	21.828182444
6.066405484	7.385536188	21.851689491

Ni(100)_Volmer

1.0

7.4579000473	0.0000000000	0.0000000000
0.0000000000	7.4579000473	0.0000000000
0.0000000000	0.0000000000	43.5157012939

Ni O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999862612
7.454207819	0.001180415	18.417444317
1.247136246	1.239990277	16.706186819
2.485941863	0.000000000	14.999862612
2.489203791	0.006422732	18.422238841
3.730625885	1.244843273	16.708110076
4.971958406	0.000000000	14.999862612

4.975348802	7.451958964	18.414982859
6.214592499	1.247737134	16.707573172
0.000000000	2.485941863	14.999862612
0.009761985	2.485914969	18.406131729
1.247865602	3.731629179	16.704590374
2.485941863	2.485941863	14.999862612
2.488888845	2.495240225	18.446591447
3.731898561	3.727494425	16.708847995
4.971958406	2.485941863	14.999862612
4.975393255	2.484968130	18.428775061
6.213506968	3.726766514	16.707736578
0.000000000	4.971958406	14.999862612
7.454310949	4.973666273	18.414408346
1.246845416	6.215042803	16.712929241
2.485941863	4.971958406	14.999862612
2.487623281	4.962137505	18.428360063
3.724879504	6.213741677	16.710248613
4.971958406	4.971958406	14.999862612
4.976904642	4.981749525	18.417479332
6.216210127	6.215106815	16.702385696
4.523097466	3.757043590	22.387568714
2.426717511	2.703968277	21.428715680
6.790033848	2.482251190	21.591794358
4.740206379	6.327035664	21.605485404
5.373853007	3.323514111	22.083258412
4.582148232	4.708908229	22.069516789

2.461581867	1.747755845	21.639274027
3.334397873	3.130625391	21.786801950
6.662041181	2.349487654	20.610963286
2.475229466	2.718237100	20.086514667
4.822171989	6.336602297	20.610064556
3.910780950	6.809048426	21.782952843
0.215895859	2.903658903	21.650524366

Ni(100)_Heyrovsky

1.0

7.4579000473	0.0000000000	0.0000000000
0.0000000000	7.4579000473	0.0000000000
0.0000000000	0.0000000000	43.5157012939

Ni H O

27 10 4

Cartesian

0.000000000	0.000000000	14.999862612
7.456046376	7.457358171	18.396894131
1.255046355	1.255386306	16.715533354
2.485941863	0.000000000	14.999862612
2.487501258	7.441382369	18.396354634
3.717581951	1.254538263	16.714587937
4.971958406	0.000000000	14.999862612
4.974405075	7.455637413	18.397660581
6.214978791	1.241939966	16.694336031
0.000000000	2.485941863	14.999862612

7.440289726	2.487121411	18.397150911
1.254324112	3.717446371	16.714823967
2.485941863	2.485941863	14.999862612
2.483550538	2.485561349	18.556224858
3.716835815	3.716920275	16.715445167
4.971958406	2.485941863	14.999862612
4.987239859	2.485167722	18.397552941
6.213726563	3.730710789	16.694546124
0.000000000	4.971958406	14.999862612
7.455409371	4.973992111	18.396492102
1.241712035	6.215291737	16.694385312
2.485941863	4.971958406	14.999862612
2.485451329	4.987407445	18.396767038
3.730944165	6.214164421	16.694578545
4.971958406	4.971958406	14.999862612
4.972471389	4.973206190	18.397730612
6.214583164	6.214885886	16.691830480
2.498656625	2.479277315	20.188091928
5.370399044	3.282391726	23.181872420
4.592867519	4.668973838	23.201914233
2.432190064	1.654750556	22.857053433
3.280366467	3.025791169	22.898363897
6.715159310	2.231816424	21.697346523
2.486736452	2.511990612	21.061280282
4.838674108	6.375031081	21.739012328
3.897981728	6.791486558	22.900195076

0.171830673	2.953340627	22.725724701
4.530897110	3.718327643	23.502038241
2.408688224	2.584053305	22.542324086
6.783732255	2.467848120	22.641812092
4.730148990	6.320581154	22.706982351

Cu(100)_Rf_sur

1.0

7.6687002182	0.0000000000	0.0000000000
0.0000000000	7.6687002182	0.0000000000
0.0000000000	0.0000000000	43.6150016785

Cu H O

27 8 4

Cartesian

0.000000000	0.000000000	15.000071048
7.667651196	0.000357286	18.537300411
1.277462645	1.277959731	16.770038201
2.556207885	0.000000000	15.000071048
2.557427402	0.006418672	18.541036118
3.833144991	1.279683418	16.770207179
5.112492562	0.000000000	15.000071048
5.110638604	7.668005898	18.534759247
6.392597759	1.276804550	16.768066361
0.000000000	2.556207885	15.000071048
0.004679435	2.557237024	18.542337246
1.278772665	3.834110137	16.770571131

2.556207885	2.556207885	15.000071048
2.559185370	2.560540186	18.541714628
3.833659446	3.833844339	16.770022603
5.112492562	2.556207885	15.000071048
5.113718477	2.556030763	18.540929532
6.392059307	3.829879996	16.766510467
0.000000000	5.112492562	15.000071048
7.666937221	5.110224480	18.536498417
1.276435221	6.392724373	16.769990107
2.556207885	5.112492562	15.000071048
2.556789990	5.113848748	18.541956396
3.829654651	6.392263626	16.766752235
5.112492562	5.112492562	15.000071048
5.109777903	5.109737679	18.533203352
6.390984231	6.390741516	16.766397382
5.576909412	3.397869923	23.312494086
4.786232124	4.760208153	23.305550403
3.207075237	3.178963507	23.016452982
7.028353939	2.239645758	21.862967114
2.517495549	2.639479198	21.722267195
5.066079170	6.487630916	21.832262569
4.087040058	6.946256891	22.943340237
0.457712281	2.786240790	22.824520329
4.723224532	3.809947437	23.596678155
2.340059094	2.817474903	22.656088572
7.156146290	2.603134132	22.757909326

4.910327529 6.443808769 22.792814916

Cu(100)_Rf_top

1.0

7.6687002182	0.0000000000	0.0000000000
0.0000000000	7.6687002182	0.0000000000
0.0000000000	0.0000000000	43.6150016785

Cu H O

27 9 4

Cartesian

0.000000000	0.000000000	15.000071048
7.668120628	0.000055399	18.515672567
1.282738837	1.282963954	16.756200228
2.556207885	0.000000000	15.000071048
2.557053502	0.014499712	18.545131877
3.827902853	1.284252034	16.754276482
5.112492562	0.000000000	15.000071048
5.110936170	7.667720674	18.512169530
6.392065706	1.282377050	16.771486210
0.000000000	2.556207885	15.000071048
0.010783760	2.556824728	18.542859777
1.284449040	3.827713617	16.755064178
2.556207885	2.556207885	15.000071048
2.560251990	2.563044126	18.586223350
3.828289551	3.828643339	16.753753951
5.112492562	2.556207885	15.000071048

5.107148263	2.556375637	18.542281353
6.392103188	3.822908914	16.771206747
0.000000000	5.112492562	15.000071048
7.668420936	5.110218995	18.512404799
1.282194100	6.393527023	16.771612293
2.556207885	5.112492562	15.000071048
2.556752508	5.109979023	18.540627972
3.822429884	6.393653637	16.771204147
5.112492562	5.112492562	15.000071048
5.109483994	5.109600095	18.509497083
6.391119530	6.390635471	16.752777780
2.575315853	2.537840860	20.112380402
5.572619621	3.394626869	23.319367578
4.782961187	4.756484697	23.313739321
3.210131570	3.183302207	23.030332549
7.029455983	2.245017710	21.860279069
2.520727633	2.640014679	21.727588693
5.060584490	6.487728276	21.835522539
4.088175927	6.950420525	22.949657403
0.450116157	2.785300784	22.833658122
4.729482553	3.813038966	23.624663460
2.344747468	2.811409545	22.671361555
7.152488197	2.588939654	22.764938797
4.910785534	6.451345728	22.799134681

Cu(100)_Rf_min

1.0

7.6687002182	0.0000000000	0.0000000000
0.0000000000	7.6687002182	0.0000000000
0.0000000000	0.0000000000	43.6150016785

Cu H O

27 9 4

Cartesian

0.000000000	0.000000000	15.000071048
7.663142002	0.001538587	18.543964631
1.280203815	1.281122909	16.770261771
2.556207885	0.000000000	15.000071048
2.560693539	0.002729178	18.529120591
3.834719438	1.280432017	16.759362711
5.112492562	0.000000000	15.000071048
5.110613007	0.001217345	18.534738450
6.385804028	1.283426872	16.770386555
0.000000000	2.556207885	15.000071048
7.665219934	2.554626810	18.544686036
1.276148854	3.833508378	16.763802924
2.556207885	2.556207885	15.000071048
2.547199324	2.551378271	18.563347671
3.836231949	3.833513634	16.726781214
5.112492562	2.556207885	15.000071048
5.118163679	2.548629102	18.572918307
6.390011543	3.833328284	16.764346253
0.000000000	5.112492562	15.000071048

7.668673707	5.103183006	18.548189073
1.278913564	6.386536287	16.772169919
2.556207885	5.112492562	15.000071048
2.553703488	5.116684992	18.557133192
3.836155158	6.389381216	16.760038621
5.112492562	5.112492562	15.000071048
5.118839258	5.116095346	18.567253656
6.389105133	6.383787804	16.771933351
3.846785704	3.811541310	18.965449569
6.818684858	4.703693070	22.287285677
6.029758682	6.067183395	22.279725876
4.457620871	4.494453653	22.066738604
0.611159187	3.619424720	20.824274287
3.709321326	3.956653721	20.805282495
6.291688252	0.128520624	20.803170274
5.332509707	0.586944722	21.937858024
1.695912796	4.094098445	21.837966216
5.976557959	5.124228808	22.594065963
3.580105139	4.108667279	21.755971744
0.733307046	3.867278427	21.769601744
6.157017608	0.089729904	21.781314497

Cu(100)_Volmer

1.0

7.6687002182	0.0000000000	0.0000000000
0.0000000000	7.6687002182	0.0000000000

0.0000000000 0.0000000000 43.6150016785

Cu O H

27 4 9

Cartesian

0.000000000	0.000000000	15.000071048
7.664259130	0.001193965	18.549618884
1.283070227	1.275451106	16.770363158
2.556207885	0.000000000	15.000071048
2.559937055	0.000672290	18.553563863
3.837574423	1.278140624	16.771469312
5.112492562	0.000000000	15.000071048
5.113308467	7.663428140	18.552317328
6.392950176	1.278049549	16.772938118
0.000000000	2.556207885	15.000071048
0.019841612	2.557483167	18.543708565
1.282003150	3.836332509	16.770528236
2.556207885	2.556207885	15.000071048
2.567688619	2.557572756	18.602766266
3.838893128	3.832210927	16.770935082
5.112492562	2.556207885	15.000071048
5.117106887	2.556556416	18.563247585
6.391657068	3.831230469	16.772253108
0.000000000	5.112492562	15.000071048
7.661033445	5.113461593	18.546947737
1.279348028	6.388616961	16.779307277
2.556207885	5.112492562	15.000071048

2.558919115	5.091607198	18.569810418
3.827502213	6.386467723	16.775137428
5.112492562	5.112492562	15.000071048
5.114360689	5.116925422	18.551321660
6.391721974	6.393076332	16.770459345
4.615137795	3.861403447	22.563221037
2.468759683	2.758105063	21.652501509
6.868063850	2.569476755	21.716781920
4.814936928	6.442722722	21.724543195
5.449665112	3.418926924	22.234793410
4.668153396	4.802428199	22.224511768
2.529844296	1.801837953	21.853896912
3.363139071	3.184607885	21.979023587
6.750138704	2.448707595	20.735879461
2.529447085	2.772673897	20.231161315
4.879606500	6.450794020	20.731409351
3.982119128	6.915896049	21.914445516
0.051509604	3.046096999	21.790592672

Cu(100)_Heyrovsky

1.0

7.6687002182	0.0000000000	0.0000000000
0.0000000000	7.6687002182	0.0000000000
0.0000000000	0.0000000000	43.6150016785

Cu H O

27 10 4

Cartesian

0.000000000	0.000000000	15.000071048
7.661016076	7.663896658	18.548129281
1.285171356	1.285296370	16.785910405
2.556207885	0.000000000	15.000071048
2.558903574	7.647827196	18.541901804
3.824421882	1.284938697	16.784348011
5.112492562	0.000000000	15.000071048
5.117884854	7.660827297	18.553927815
6.389976347	1.274381058	16.772513074
0.000000000	2.556207885	15.000071048
7.647112307	2.557714911	18.548283961
1.284844765	3.820622778	16.783688998
2.556207885	2.556207885	15.000071048
2.556065730	2.558068699	18.666001615
3.824387601	3.822337094	16.781709360
5.112492562	2.556207885	15.000071048
5.127664298	2.557372322	18.547813423
6.388294255	3.840023055	16.772253108
0.000000000	5.112492562	15.000071048
7.661396375	5.115529926	18.544839416
1.273589720	6.391440864	16.772145223
2.556207885	5.112492562	15.000071048
2.557640863	5.124572540	18.539719392
3.841711089	6.390331506	16.772225812
5.112492562	5.112492562	15.000071048

5.115695392	5.117481243	18.553177814
6.392283738	6.392618328	16.769568963
2.607619100	2.528993195	20.287849429
5.437142671	3.342783475	23.150527675
4.643627310	4.739226344	23.163775526
2.516743179	1.777185367	22.851819324
3.463585089	3.157491469	22.896320247
6.819467853	2.329308334	21.719476464
2.595261439	2.617668227	21.312160955
4.926139192	6.442411444	21.749174942
4.004522944	6.869156295	22.926770025
7.646453640	3.121509103	22.770190104
4.585061263	3.778541001	23.452077452
2.553408894	2.697296760	22.505422870
6.860797488	2.550144127	22.670859822
4.806579035	6.355332570	22.715581715

Au(100)_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
0.0000000000	8.6400995255	0.0000000000
0.0000000000	0.0000000000	44.0730018616

Au H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999804945
-------------	-------------	--------------

8.638605539	8.639797226	19.220943032
1.442535576	1.446551597	17.123010302
2.880004422	0.000000000	14.999804945
2.879034695	0.009928477	19.222349767
4.313927303	1.447111906	17.121821605
5.760095361	0.000000000	14.999804945
5.761817488	8.640037212	19.215553832
7.199889645	1.441275781	17.107131669
0.000000000	2.880004422	14.999804945
8.632331930	2.880800339	19.228201310
1.443476977	4.316679925	17.123757671
2.880004422	2.880004422	14.999804945
2.872382311	2.890468762	19.271011493
4.314821326	4.318136317	17.122558466
5.760095361	2.880004422	14.999804945
5.753949470	2.881385367	19.222067369
7.200752768	4.319950627	17.107381229
0.000000000	5.760095361	14.999804945
8.638819260	5.763044709	19.219222376
1.440550804	7.201399081	17.107499442
2.880004422	5.760095361	14.999804945
2.879815420	5.770194832	19.225020067
4.319081581	7.202538239	17.107140863
5.760095361	5.760095361	14.999804945
5.761045518	5.762097128	19.216022744
7.200860401	7.200881516	17.106221429

5.861041654	3.699059810	23.964473573
5.110274720	5.094112787	23.992374468
3.642554328	3.387374949	23.748642899
7.220605635	2.607281649	22.467416223
2.803473036	2.911504304	22.515964990
5.323146893	6.839680875	22.524379129
4.344513336	7.226640289	23.661186292
8.049590805	3.443096101	23.477985034
5.057871906	4.159348916	24.327899748
2.793386955	2.919818303	23.477987661
7.291173179	2.832930725	23.413742835
5.197587680	6.785372083	23.490229274

Au(100)_Rf_top

1.0

8.6400995255	0.0000000000	0.0000000000
0.0000000000	8.6400995255	0.0000000000
0.0000000000	0.0000000000	44.0730018616

Au H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999804945
8.632285066	8.633652365	19.227268741
1.450755718	1.453191235	17.126924466
2.880004422	0.000000000	14.999804945
2.879535008	8.621730345	19.219239451

4.307931532	1.452778213	17.124071592
5.760095361	0.000000000	14.999804945
5.768555618	8.632924684	19.221599771
7.199854626	1.435626984	17.106405315
0.000000000	2.880004422	14.999804945
8.604064126	2.881284172	19.224886092
1.454940013	4.305564380	17.130474796
2.880004422	2.880004422	14.999804945
2.866649184	2.897812263	19.316734969
4.306570670	4.308968979	17.127251522
5.760095361	2.880004422	14.999804945
5.781445304	2.881636425	19.217014420
7.200852161	4.327080922	17.105387370
0.000000000	5.760095361	14.999804945
8.633621980	5.768391851	19.225613759
1.434065405	7.201596837	17.106196472
2.880004422	5.760095361	14.999804945
2.879811300	5.799378288	19.222780587
4.324943198	7.202894097	17.105929836
5.760095361	5.760095361	14.999804945
5.766337041	5.768484035	19.221699595
7.201866692	7.199520397	17.095675515
2.931264472	2.801741124	20.924699758
5.860468470	3.698200034	23.962779186
5.111373709	5.094545893	23.990238753
3.644725526	3.387510906	23.753526409

7.220314151	2.610419741	22.470358413
2.805592220	2.912130532	22.519574427
5.321885167	6.836973573	22.526112919
4.344968072	7.223119817	23.665100456
8.043781202	3.446430920	23.485109338
5.059681066	4.160980920	24.329100267
2.794465602	2.920622203	23.492801064
7.288081178	2.832208451	23.417557174
5.200096712	6.784640282	23.492023485

Au(100)_Rf_min

1.0

8.6400995255	0.0000000000	0.0000000000
0.0000000000	8.6400995255	0.0000000000
0.0000000000	0.0000000000	44.0730018616

Au H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999804945
8.632915414	0.000587122	19.244481868
1.436708721	1.447808301	17.121900413
2.880004422	0.000000000	14.999804945
2.882979262	8.634553082	19.208856409
4.329101743	1.445016927	17.122608378
5.760095361	0.000000000	14.999804945
5.760006783	8.639594835	19.277199286

7.197223541	1.425380870	17.105879924
0.000000000	2.880004422	14.999804945
8.621038198	2.869816373	19.229975819
1.438491230	4.317559786	17.117844394
2.880004422	2.880004422	14.999804945
2.881019982	2.793294772	19.274208498
4.323190687	4.319135913	17.123736655
5.760095361	2.880004422	14.999804945
5.780249498	2.866372635	19.229831336
7.199279382	4.319605326	17.119633350
0.000000000	5.760095361	14.999804945
8.622275204	5.769687566	19.220047240
1.438298109	7.190918003	17.119156558
2.880004422	5.760095361	14.999804945
2.879419908	5.836116135	19.276164266
4.327577887	7.193017618	17.122544017
5.760095361	5.760095361	14.999804945
5.778170483	5.774289003	19.229315139
7.196091593	7.215910471	17.104756901
2.905420984	4.314188403	20.160279315
5.839583048	5.226951384	23.275522938
5.092134195	6.624043206	23.302701421
3.617275783	4.916637941	23.116166556
7.199517307	4.167046215	21.727002214
2.740023685	4.429637073	21.913095750
5.275990282	8.357248958	21.791504482

4.329655872	0.122544050	22.955612282
8.027966372	4.950144225	22.779777008
5.053877643	5.697035858	23.664107467
2.760296011	4.454406035	22.881918296
7.272245234	4.335802794	22.690794140
5.183445538	8.320388029	22.772755155

Au(100)_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
0.0000000000	8.6400995255	0.0000000000
0.0000000000	0.0000000000	44.0730018616

Au O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999804945
8.635850342	8.634237394	19.221212295
1.450553713	1.450744903	17.115635124
2.880004422	0.000000000	14.999804945
2.878355681	8.632937044	19.210556049
4.310417131	1.450334714	17.119328624
5.760095361	0.000000000	14.999804945
5.763646218	8.629356318	19.233941208
7.197286885	1.432553523	17.107888232
0.000000000	2.880004422	14.999804945
8.629096763	2.877804641	19.207708429

1.450711043	4.310115089	17.115942478
2.880004422	2.880004422	14.999804945
2.878056987	2.883435543	19.342849534
4.312641116	4.310695741	17.115163585
5.760095361	2.880004422	14.999804945
5.767482894	2.875958917	19.214671175
7.200670885	4.323069149	17.105438596
0.000000000	5.760095361	14.999804945
8.637413337	5.764967682	19.218532800
1.437169765	7.199784072	17.106197786
2.880004422	5.760095361	14.999804945
2.882537915	5.769816829	19.209647123
4.324344780	7.202408976	17.107506010
5.760095361	5.760095361	14.999804945
5.768277009	5.763329499	19.220887866
7.201085967	7.201486114	17.098607198
5.120778457	4.086771624	23.348512900
2.891302789	2.888155427	22.593822700
7.300959535	2.727703835	22.419453267
5.228000933	6.684472140	22.465958263
5.913881694	3.621720405	22.959079864
5.147822645	5.014555577	22.983765366
3.042282168	1.932061311	22.722543526
3.772346758	3.343214551	22.840622554
7.245648572	2.670989010	21.431426362
2.889418440	2.934867085	20.975160948

5.343302059	6.657547945	21.481226873
4.362448895	7.117404717	22.596302546
8.074494179	3.301504991	22.582471625

Au(100)_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
0.0000000000	8.6400995255	0.0000000000
0.0000000000	0.0000000000	44.0730018616

Au H O

27 10 4

Cartesian

0.000000000	0.000000000	14.999804945
8.631027461	8.632370555	19.226991597
1.454802381	1.457395099	17.145490475
2.880004422	0.000000000	14.999804945
2.879084649	8.610426313	19.204996098
4.305135651	1.457236739	17.144456768
5.760095361	0.000000000	14.999804945
5.767854202	8.631757716	19.229001218
7.199999853	1.432147582	17.099455704
0.000000000	2.880004422	14.999804945
8.606157045	2.879527026	19.216616436
1.455821933	4.302925313	17.144811407
2.880004422	2.880004422	14.999804945
2.877187168	2.881735818	19.366054747

4.307448471	4.306480547	17.143227352
5.760095361	2.880004422	14.999804945
5.791105488	2.881401332	19.210986870
7.200364981	4.328990505	17.099573917
0.000000000	5.760095361	14.999804945
8.631119129	5.768362497	19.221957037
1.430986151	7.200875851	17.096936454
2.880004422	5.760095361	14.999804945
2.880383454	5.792710197	19.204524559
4.329785650	7.201304323	17.098106763
5.760095361	5.760095361	14.999804945
5.766957604	5.770269505	19.232590953
7.199542542	7.200980394	17.103149204
2.911095144	2.891640880	21.124055479
5.841314959	3.685671871	23.964696864
5.047947018	5.081509950	23.979586448
2.955791389	2.072242894	23.702093245
3.859622382	3.476866832	23.738797069
7.187892436	2.672532177	22.515287235
2.949983846	2.945266795	22.167189346
5.324471447	6.786975247	22.559638127
4.388622750	7.216736515	23.721204347
8.024989214	3.465695410	23.554497744
4.995778524	4.125529004	24.281313317
2.954604852	2.999810937	23.374735171
7.248108165	2.881065816	23.467574409

5.201136477 6.712549398 23.525672160

Ag(100)_Rf_sur

1.0

8.6679000854	0.0000000000	0.0000000000
0.0000000000	8.6679000854	0.0000000000
0.0000000000	0.0000000000	44.0861015320

Ag H O

27 8 4

Cartesian

0.000000000	0.000000000	14.999855259
0.001128853	0.001494028	19.108541884
1.446544731	1.447455968	17.054424557
2.889271182	0.000000000	14.999855259
2.890512685	0.006819627	19.128956768
4.328985322	1.447602696	17.053586309
5.778629161	0.000000000	14.999855259
5.779233122	0.000656799	19.103735754
7.222052828	1.447919400	17.052864995
0.000000000	2.889271182	14.999855259
8.663718860	2.890494344	19.120210347
1.446663302	4.333219762	17.053712440
2.889271182	2.889271182	14.999855259
2.882064214	2.893779703	19.134326548
4.328668359	4.332021916	17.051984704
5.778629161	2.889271182	14.999855259

5.768047712	2.889685792	19.120459982
7.222665571	4.330144678	17.051537988
0.000000000	5.778629161	14.999855259
0.001606418	5.777798910	19.108290935
1.449516486	7.224651563	17.056411126
2.889271182	5.778629161	14.999855259
2.890875372	5.779843282	19.127872827
4.329443072	7.224592665	17.054286601
5.778629161	5.778629161	14.999855259
5.779650056	5.775789669	19.098838967
7.225253973	7.223465341	17.044265728
5.855559982	3.700598556	23.891426842
5.109161459	5.100370708	23.918019535
3.641204288	3.384998472	23.617863714
7.240385534	2.568402073	22.439260864
2.854655310	2.905388764	22.354442787
5.335756163	6.868339686	22.479914574
4.330682766	7.221390486	23.604814375
8.040445609	3.466453571	23.420405089
5.040340964	4.158649613	24.231645132
2.803258481	2.916128824	23.314717530
7.293429692	2.840372342	23.373565687
5.192870173	6.793535902	23.440047418

Ag(100)_Rf_top

1.0

8.6679000854	0.0000000000	0.0000000000
0.0000000000	8.6679000854	0.0000000000
0.0000000000	0.0000000000	44.0861015320

Ag H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999855259
8.667545149	0.000436730	19.090928167
1.450545001	1.451048473	17.041681349
2.889271182	0.000000000	14.999855259
2.890397215	0.003033062	19.124148010
4.326786472	1.449575512	17.039421496
5.778629161	0.000000000	14.999855259
5.780964406	8.666601751	19.085346854
7.221128546	1.450627923	17.055203681
0.000000000	2.889271182	14.999855259
8.658914559	2.890264436	19.112437503
1.451609035	4.328196919	17.041756240
2.889271182	2.889271182	14.999855259
2.878165594	2.895545086	19.136176474
4.325619883	4.328660093	17.038599014
5.778629161	2.889271182	14.999855259
5.771281923	2.889434185	19.113769765
7.221785204	4.327832941	17.053645433
0.000000000	5.778629161	14.999855259
0.000735371	5.778853386	19.090082036

1.451709265	7.225526246	17.058694629
2.889271182	5.778629161	14.999855259
2.890730969	5.784854759	19.120666260
4.326167529	7.225399151	17.056782950
5.778629161	5.778629161	14.999855259
5.780705049	5.777694547	19.080342330
7.226224236	7.223063389	17.034612738
2.976962212	2.839809972	20.809618881
5.857540290	3.700888137	23.892937791
5.116554679	5.104459970	23.920739242
3.639726936	3.380232660	23.623949552
7.240106027	2.574324398	22.434657069
2.858956913	2.907757591	22.349300307
5.333084580	6.863718278	22.476708735
4.332867150	7.216911156	23.606372623
8.030966168	3.469629917	23.425613262
5.042273224	4.161383968	24.228497104
2.800848839	2.915529513	23.327511978
7.291953631	2.835647604	23.372469921
5.195206451	6.794329472	23.439603331

Ag(100)_Rf_min

1.0

8.6679000854	0.0000000000	0.0000000000
0.0000000000	8.6679000854	0.0000000000
0.0000000000	0.0000000000	44.0861015320

Ag H O

27 9 4

Cartesian

0.000000000	0.000000000	14.999855259
8.655335744	8.664697907	19.116941443
1.450632314	1.446530136	17.057743388
2.889271182	0.000000000	14.999855259
2.892349882	0.000826166	19.108231811
4.330488765	1.458483413	17.045247187
5.778629161	0.000000000	14.999855259
5.762753113	0.007039390	19.084872548
7.215033660	1.453536646	17.052788791
0.000000000	2.889271182	14.999855259
8.667650545	2.887123739	19.095842034
1.455288080	4.334544187	17.045795070
2.889271182	2.889271182	14.999855259
2.884238781	2.886385708	19.139875013
4.336530178	4.335477252	17.009933038
5.778629161	2.889271182	14.999855259
5.785473186	2.889819603	19.153306688
7.211705936	4.335023119	17.047826311
0.000000000	5.778629161	14.999855259
8.667134931	5.765888644	19.110182905
1.448967806	7.216701397	17.064042072
2.889271182	5.778629161	14.999855259
2.887986798	5.782345404	19.142121728

4.330508398	7.212635901	17.045060618
5.778629161	5.778629161	14.999855259
5.786298788	5.790500162	19.151469900
7.217762073	7.213382973	17.057464848
4.354330221	4.331371199	19.558000432
7.275831658	5.224249768	22.768826310
6.521483486	6.618885415	22.793009368
5.053006568	4.907539926	22.566685058
8.648848723	4.124215342	21.318219893
4.221949992	4.385546556	21.351946890
6.769718987	8.378256868	21.366897396
5.752613396	0.088812170	22.482421434
0.818849755	4.959963074	22.324286884
6.465074921	5.681484523	23.117942116
4.200160400	4.436443529	22.319394039
0.054779047	4.348770065	22.273850111
6.620298961	8.326337968	22.337756661

Ag(100)_Volmer

1.0

8.6679000854	0.0000000000	0.0000000000
0.0000000000	8.6679000854	0.0000000000
0.0000000000	0.0000000000	44.0861015320

Ag O H

27 4 9

Cartesian

0.000000000	0.000000000	14.999855259
8.664359503	8.664446816	19.139336327
1.450109984	1.445335390	17.059027037
2.889271182	0.000000000	14.999855259
2.890935044	8.667367422	19.140964210
4.328405386	1.443026235	17.061281635
5.778629161	0.000000000	14.999855259
5.782616644	8.652658479	19.156969752
7.223127454	1.438136558	17.072890975
0.000000000	2.889271182	14.999855259
0.009599169	2.888120351	19.127516769
1.450670804	4.331219304	17.059295066
2.889271182	2.889271182	14.999855259
2.889450459	2.883713351	19.204452949
4.329057911	4.326747982	17.052443244
5.778629161	2.889271182	14.999855259
5.772383931	2.882410109	19.117996480
7.228640595	4.331666979	17.063608496
0.000000000	5.778629161	14.999855259
8.667054851	5.784418192	19.133117789
1.448871322	7.220911554	17.077731265
2.889271182	5.778629161	14.999855259
2.899171433	5.761923894	19.144368442
4.333514768	7.222023379	17.074824989
5.778629161	5.778629161	14.999855259
5.790964628	5.773512805	19.118997647

7.225067980	7.225817635	17.057091709
4.957290459	4.165731553	23.236862955
2.754990208	2.973686670	22.459573266
7.186127771	2.832900075	22.337118121
5.102601074	6.784431030	22.375822051
5.759194447	3.698993075	22.869305695
5.002981695	5.096486555	22.881451093
2.882945614	2.016495869	22.617405627
3.639444588	3.426525274	22.723229828
7.130577874	2.721055276	21.355041050
2.788761879	2.994057032	20.926470378
5.184014841	6.819795008	21.390418265
4.255251772	7.232285024	22.565321263
7.948977372	3.429695938	22.467632534

Ag(100)_Heyrovsky

1.0

8.6679000854	0.0000000000	0.0000000000
0.0000000000	8.6679000854	0.0000000000
0.0000000000	0.0000000000	44.0861015320

Ag H O

27 10 4

Cartesian

0.000000000	0.000000000	14.999855259
8.656708992	8.657460197	19.136709904
1.455047064	1.455651541	17.083495205

2.889271182	0.000000000	14.999855259
2.889909758	8.647495625	19.122688303
4.323669024	1.454442587	17.082090680
5.778629161	0.000000000	14.999855259
5.789986615	8.655800727	19.138170926
7.222112242	1.438628535	17.059618278
0.000000000	2.889271182	14.999855259
8.645083399	2.889751406	19.123470054
1.455147939	4.323361102	17.083760606
2.889271182	2.889271182	14.999855259
2.886407924	2.889908208	19.231224328
4.323270689	4.324099649	17.081530972
5.778629161	2.889271182	14.999855259
5.797109112	2.889807979	19.121907865
7.222558625	4.339741657	17.058864118
0.000000000	5.778629161	14.999855259
8.656640795	5.789216294	19.137809612
1.438932970	7.222729119	17.060572146
2.889271182	5.778629161	14.999855259
2.890370091	5.798993840	19.125552536
4.339650727	7.222965743	17.059819300
5.778629161	5.778629161	14.999855259
5.790189140	5.789075249	19.136298664
7.224088934	7.223263848	17.050836383
2.935124905	2.889461567	21.004745391
5.831710002	3.675075672	23.838535763

5.022100222	5.078828590	23.855815758
2.942911551	2.088949942	23.586932629
3.922324378	3.508706779	23.634865169
7.188312155	2.652481998	22.433393128
2.970297206	2.952922364	22.119536290
5.334615923	6.786391706	22.477565377
4.386481170	7.210399336	23.634026921
8.013935929	3.468388673	23.468214125
4.975034704	4.113050081	24.144036400
2.974761812	3.011256214	23.246259740
7.224330208	2.901665546	23.376085686
5.181701812	6.680236225	23.435454135

Single-Atom Alloy(111)

Pt@Au_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pt H O

26 1 8 4

Cartesian

0.010459287	0.351534715	22.982575893
1.439816364	1.148814094	20.449080467
-0.000043130	1.995370371	17.999999523
2.869797544	0.351626116	22.983047962

4.323386705	1.161724965	20.481851101
2.880047681	1.995370371	17.999999523
5.759869393	0.332454792	22.970092297
7.196717564	1.161768784	20.481710434
5.760052102	1.995370371	17.999999523
-1.418367768	2.826120270	22.983219624
-0.012963974	3.665583340	20.449581146
-1.440045470	4.489527587	17.999999523
2.892821494	3.665230336	20.449187756
1.440045341	4.489527587	17.999999523
4.298425201	2.826464355	22.982723713
5.760255395	3.655837469	20.499773026
4.320049763	4.489527587	17.999999523
-2.879541156	5.320740874	22.987513542
-1.438319609	6.152981732	20.499942303
-2.880047552	6.983684356	17.999999523
0.011632596	5.302316396	22.984058857
1.439989465	6.155851261	20.481820107
0.000043259	6.983684356	17.999999523
2.869072985	5.303249862	22.982847691
4.318640492	6.152793076	20.498557091
2.880047681	6.983684356	17.999999523
1.440042509	2.826742879	22.742750645
1.034302566	3.548993694	27.135863304
-0.694159226	4.919499266	27.589905262
2.360715221	7.235772030	27.301993370

0.656363075	5.753457203	27.577323914
1.472755450	2.800493428	25.827770233
-2.539510888	4.710173096	26.270091534
-2.746790204	5.813581719	27.341158390
5.580301371	0.013356001	26.240217686
0.261978020	4.886388636	27.864062786
1.393857685	7.301351504	27.187273502
1.494746169	2.723729081	26.792399883
-2.404074778	4.908613433	27.215812206

Pt@Au_Rf_top

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pt H O

26 1 9 4

Cartesian

0.002227944	0.335610203	22.953016758
1.440077399	1.170418401	20.470008850
-0.000043130	1.995370371	17.999999523
2.879186505	0.336085577	22.952356339
4.320653782	1.163776317	20.469071865
2.880047681	1.995370371	17.999999523
5.761347721	0.333719103	22.910521030
7.200171151	1.163303785	20.469264984

5.760052102	1.995370371	17.999999523
-1.436786050	2.827594728	22.949266434
0.005245431	3.655319223	20.467805862
-1.440045470	4.489527587	17.999999523
2.875736828	3.655555601	20.467321873
1.440045341	4.489527587	17.999999523
4.317538800	2.827528052	22.949805260
5.760475424	3.655841706	20.474491119
4.320049763	4.489527587	17.999999523
-2.880193181	5.323213467	22.928326130
-1.437205428	6.154115004	20.474486351
-2.880047552	6.983684356	17.999999523
0.000675152	5.319646849	22.952027321
1.439998992	6.152305159	20.469963551
0.000043259	6.983684356	17.999999523
2.879023108	5.319847101	22.951729298
4.317936501	6.153951770	20.473794937
2.880047681	6.983684356	17.999999523
1.440737359	2.829242009	22.842466831
1.437665186	2.857498881	24.410128593
1.030831405	3.553689793	27.325038910
-0.693781738	4.917570786	27.862017155
2.363729201	7.239806050	27.566566467
0.660277257	5.749265747	27.848677635
1.475267829	2.792423604	26.025059223
-2.543641221	4.705798336	26.543188095

-2.755645522	5.815363467	27.604780197
5.578500626	0.020111623	26.513056755
0.269146682	4.872485204	28.109843731
1.396787206	7.300533104	27.456481457
1.494822388	2.726534833	26.992554665
-2.406241405	4.912870450	27.485702038

Pt@Au_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pt H O

26 1 9 4

Cartesian

0.017959297	0.325037346	22.934391499
1.446418923	1.154197916	20.440030098
-0.000043130	1.995370371	17.999999523
2.904640130	0.286527591	22.968375683
4.330327741	1.158953555	20.464582443
2.880047681	1.995370371	17.999999523
5.795923204	0.311629749	22.941176891
7.203368918	1.159379592	20.468740463
5.760052102	1.995370371	17.999999523
-1.417733010	2.827004677	22.958734035
-0.006146278	3.660127713	20.453772545

-1.440045470	4.489527587	17.999999523
2.891505695	3.656110641	20.442748070
1.440045341	4.489527587	17.999999523
4.375480589	2.829266984	22.973001003
5.759382100	3.650331890	20.483088493
4.320049763	4.489527587	17.999999523
-2.854852725	5.307175506	22.972478867
-1.434481389	6.157483154	20.479657650
-2.880047552	6.983684356	17.999999523
0.011279312	5.303686937	22.940552235
1.446691030	6.151698160	20.465719700
0.000043259	6.983684356	17.999999523
2.894678806	5.307702671	22.934741974
4.330535990	6.146033138	20.483019352
2.880047681	6.983684356	17.999999523
1.412306431	2.840342142	22.775843143
2.627374759	2.149573408	23.708188534
2.457912386	2.675716661	26.789023876
0.702635447	4.077979939	27.070996761
3.775442621	6.408178880	26.731691360
2.048212556	4.910874179	27.059106827
2.932465751	1.833126389	25.563831329
-1.103828800	3.896695226	25.638873577
-1.384818579	4.932284144	26.758995056
2.722309314	6.595669160	25.610466003
1.639689994	4.072954027	27.401597500

2.813198881	6.468211075	26.578788757
2.942253202	1.836186246	26.531395912
-1.026553897	4.037060391	26.607260704

Pt@Au_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pt O H

26 1 4 9

Cartesian

0.003992300	0.349971253	22.922360897
1.436404168	1.168080163	20.439815521
-0.000043130	1.995370371	17.999999523
2.864716427	0.353464003	22.891590595
4.322599350	1.164923526	20.447049141
2.880047681	1.995370371	17.999999523
5.755146017	0.330282604	22.912251949
7.196272612	1.162402096	20.453844070
5.760052102	1.995370371	17.999999523
-1.426565058	2.826480411	22.909352779
0.001640887	3.658207038	20.441629887
-1.440045470	4.489527587	17.999999523
2.876230188	3.659421481	20.443007946
1.440045599	4.489527587	17.999999523

4.299494707	2.833548754	22.910327911
5.759136192	3.658925758	20.456702709
4.320049763	4.489527587	17.999999523
-2.885941452	5.321478549	22.920341492
-1.441086007	6.151838648	20.456695557
-2.880047423	6.983684356	17.999999523
0.008644881	5.310836228	22.910537720
1.440958676	6.155485545	20.450434685
0.000043517	6.983684356	17.999999523
2.869593382	5.311051644	22.926805019
4.316654433	6.154738950	20.466773510
2.880047681	6.983684356	17.999999523
1.432068660	2.829607501	22.850255966
-0.634985709	4.156685476	26.750657558
1.418510388	2.890573831	25.908181667
-0.644925146	6.773984888	26.013028622
5.655463414	2.996064013	26.031913757
-0.668748071	5.103430957	26.427223682
-1.480785561	3.724062359	26.434836388
2.201103321	3.444560742	26.103899479
0.576938475	3.440813943	26.202759743
-1.559571187	7.114309894	26.063578129
-0.443507897	6.796273908	25.042510033
1.402326954	2.851462123	24.544982910
5.557929060	3.101611951	25.050275326
5.690349098	2.028760417	26.161713600

Pt@Au⁻_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pt H O

26 1 10 4

Cartesian

-0.005605361	0.328071921	22.952356339
1.439413963	1.169303861	20.485203266
-0.000043130	1.995370371	17.999999523
2.882230627	0.330024039	22.950699329
4.325837092	1.160668739	20.473456383
2.880047681	1.995370371	17.999999523
5.757847671	0.331598260	22.983887196
7.194132893	1.160238911	20.474319458
5.760052102	1.995370371	17.999999523
-1.447841776	2.824901144	22.949767113
0.002806310	3.655901692	20.484769344
-1.440045470	4.489527587	17.999999523
2.874023842	3.655391698	20.485732555
1.440045599	4.489527587	17.999999523
4.322096462	2.824796782	22.950646877
5.758679010	3.660416940	20.472323895
4.320049763	4.489527587	17.999999523

-2.880867963	5.320030851	22.982373238
-1.441843944	6.151407372	20.474362373
-2.880047423	6.983684356	17.999999523
-0.002084165	5.326430871	22.954528332
1.439762869	6.158483520	20.474882126
0.000043517	6.983684356	17.999999523
2.879653713	5.325045166	22.951955795
4.321608895	6.151166981	20.474934578
2.880047681	6.983684356	17.999999523
1.433872413	2.825245229	22.844793797
1.475333362	2.852683924	24.606561661
0.769413308	3.600464133	27.268183231
-0.918578248	4.882599913	27.604951859
0.429127315	5.736105342	27.580118179
1.349410309	2.814225821	25.490214825
2.131013302	2.744938349	27.270848751
5.876735461	4.639482526	26.318941116
-2.995041582	5.741920664	27.385728359
5.193150136	0.097636003	26.306123734
2.001360048	7.405043436	27.357432842
0.047605424	4.856899481	27.855093479
1.210372648	2.726379849	26.933050156
-2.616671672	4.850680534	27.260379791
1.034503026	7.339919768	27.238235474

Rh@Au_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Rh H O

26 1 8 4

Cartesian

0.019466061	0.365528405	22.973496914
1.439732227	1.153786821	20.439391136
-0.000043130	1.995370371	17.999999523
2.860123568	0.365792489	22.971329689
4.323561094	1.162007168	20.470414162
2.880047681	1.995370371	17.999999523
5.760244596	0.331895013	22.957050800
7.197506850	1.161278524	20.470347404
5.760052102	1.995370371	17.999999523
-1.401303942	2.826167100	22.969417572
-0.008407213	3.662994119	20.438504219
-1.440045470	4.489527587	17.999999523
2.888310696	3.662652488	20.439174175
1.440045341	4.489527587	17.999999523
4.281269209	2.826604620	22.970840931
5.760346934	3.656487952	20.494835377
4.320049763	4.489527587	17.999999523
-2.879333068	5.321244401	22.983503342
-1.438332098	6.153187782	20.494816303

-2.880047552	6.983684356	17.999999523
0.020018179	5.287050451	22.971789837
1.440429524	6.155231774	20.471076965
0.000043259	6.983684356	17.999999523
2.861396543	5.286905949	22.972557545
4.319172735	6.152559821	20.494432449
2.880047681	6.983684356	17.999999523
1.439870631	2.826541512	22.692596912
1.034070177	3.547392797	27.064335346
-0.689935664	4.915761833	27.629883289
2.366552119	7.240232867	27.333610058
0.659991438	5.745486836	27.616293430
1.467029147	2.809671771	25.744647980
-2.544192196	4.707414174	26.309330463
-2.757143242	5.818800300	27.371680737
5.580271487	0.017935497	26.278007030
0.270319572	4.871363082	27.886049747
1.398711724	7.306039352	27.224931717
1.491508942	2.726812687	26.708402634
-2.410412117	4.913937715	27.254114151

Rh@Au_Rf_top

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Rh H O

26 1 9 4

Cartesian

0.016052836	0.360077739	22.964365482
1.439954059	1.164034213	20.439815521
-0.000043130	1.995370371	17.999999523
2.864198250	0.359984610	22.964539528
4.322392839	1.162950446	20.477168560
2.880047681	1.995370371	17.999999523
5.760780202	0.334105334	22.931423187
7.197811724	1.162852885	20.476396084
5.760052102	1.995370371	17.999999523
-1.409081483	2.828118995	22.962155342
0.000443149	3.658711011	20.438890457
-1.440045470	4.489527587	17.999999523
2.880301442	3.658564725	20.439031124
1.440045341	4.489527587	17.999999523
4.289602391	2.828397295	22.963445187
5.760283719	3.656374446	20.488147736
4.320049763	4.489527587	17.999999523
-2.879734261	5.323745093	22.951245308
-1.437874272	6.153846069	20.487601757
-2.880047552	6.983684356	17.999999523
0.015203022	5.295372708	22.964475155
1.440074438	6.155502493	20.476670265
0.000043259	6.983684356	17.999999523

2.866069048	5.296143386	22.963850498
4.318182151	6.153558403	20.486688614
2.880047681	6.983684356	17.999999523
1.440937561	2.828813185	22.751836777
1.438498440	2.849095453	24.310295582
1.032625759	3.551282092	27.169651985
-0.692474693	4.919291879	27.715866566
2.363450591	7.238965796	27.420613766
0.657233666	5.749960161	27.702670097
1.473821479	2.793853908	25.862746239
-2.542852867	4.705772915	26.395545006
-2.753231764	5.815003103	27.459442616
5.578757310	0.018426276	26.364588737
0.267467042	4.876578988	27.972817421
1.396836902	7.302817042	27.310843468
1.494851871	2.726355766	26.834528446
-2.406241373	4.911935200	27.340414524

Rh@Au_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Rh H O

26 1 9 4

Cartesian

0.026726117	0.336419153	22.959113121
1.444676132	1.158349790	20.445790291
-0.000043130	1.995370371	17.999999523
2.889782071	0.298686878	22.992284298
4.329350290	1.159043646	20.481963158
2.880047681	1.995370371	17.999999523
5.800725454	0.309150075	22.950036526
7.203341237	1.162560201	20.474221706
5.760052102	1.995370371	17.999999523
-1.390119533	2.821372213	22.971439362
-0.009776829	3.662755958	20.448861122
-1.440045470	4.489527587	17.999999523
2.887557781	3.657778660	20.448133945
1.440045341	4.489527587	17.999999523
4.356256912	2.835409443	22.994189262
5.756153112	3.651742125	20.493519306
4.320049763	4.489527587	17.999999523
-2.845108212	5.300292473	22.996580601
-1.437314091	6.159240373	20.492599010
-2.880047552	6.983684356	17.999999523
0.030803101	5.282287676	22.955477238
1.444475286	6.150830701	20.473198891
0.000043259	6.983684356	17.999999523
2.890449450	5.295886939	22.966418266
4.327997089	6.147281923	20.498056412
2.880047681	6.983684356	17.999999523

1.454353310	2.817439434	22.721054554
2.626738488	2.145904657	23.720972538
2.458032121	2.672254852	26.890299320
0.707598922	4.075422160	27.191097736
3.779237325	6.402498248	26.858487129
2.059545943	4.901540407	27.177672386
2.927315336	1.848282173	25.645837784
-1.125139475	3.875506474	25.789539814
-1.377118834	4.940290637	26.889395714
2.703828381	6.625884394	25.763590336
1.646650085	4.063923531	27.517864704
2.816013559	6.464862994	26.723730564
2.940093655	1.836772617	26.614484787
-1.024002250	4.042385565	26.750204563

Rh@Au_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au	Rh	O	H
26	1	4	9

Cartesian

0.012575060	0.367319156	22.936463356
1.436603212	1.165360489	20.435128212
-0.000043130	1.995370371	17.999999523

2.854536039	0.372807341	22.909111977
4.324057930	1.164878703	20.453050137
2.880047681	1.995370371	17.999999523
5.752773023	0.333461513	22.939608097
7.194917158	1.161448560	20.459933281
5.760052102	1.995370371	17.999999523
-1.406961591	2.827249974	22.924706936
-0.001467593	3.661111800	20.436491966
-1.440045470	4.489527587	17.999999523
2.880237841	3.662976057	20.438253880
1.440045599	4.489527587	17.999999523
4.279147192	2.836001278	22.923817635
5.760203638	3.660366543	20.466866493
4.320049763	4.489527587	17.999999523
-2.886290455	5.322581047	22.942204475
-1.442049554	6.152404615	20.468139648
-2.880047423	6.983684356	17.999999523
0.018501790	5.296582691	22.923200130
1.441442767	6.158484412	20.457007885
0.000043517	6.983684356	17.999999523
2.860061946	5.297897483	22.943258286
4.318631995	6.154554309	20.474703312
2.880047681	6.983684356	17.999999523
1.430166673	2.831506323	22.759864330
-0.611923424	4.140662233	26.738855839
1.419277594	2.888329364	25.817716122

-0.637818026	6.773164258	26.048271656
5.650818590	2.987863290	26.068143845
-0.654824027	5.093116888	26.434745789
-1.466428604	3.714400335	26.440200806
2.204630874	3.445258947	25.994434357
0.584394244	3.435672964	26.134996414
-1.551159855	7.115718345	26.099088192
-0.428703220	6.810024810	25.080835819
1.380963879	2.846960254	24.447979927
5.527389634	3.097512370	25.090556145
5.698266556	2.020830635	26.192107201

Rh@Au⁻_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Rh H O

26 1 10 4

Cartesian

-0.000043130	1.995370371	17.999999523
2.880047681	1.995370371	17.999999523
5.760052102	1.995370371	17.999999523
-1.440045470	4.489527587	17.999999523
1.440045341	4.489527587	17.999999523
4.320049763	4.489527587	17.999999523

-2.880047552	6.983684356	17.999999523
0.000043259	6.983684356	17.999999523
2.880047681	6.983684356	17.999999523
0.006177676	0.346815982	22.979199886
1.439397355	1.173936628	20.487198830
2.868469755	0.349210414	22.979199886
4.322425605	1.163460998	20.476799011
5.757027727	0.331252307	22.952399254
7.197073293	1.162712731	20.476799011
-1.426221286	2.825558986	22.978401184
0.006004913	3.654400475	20.486400127
2.870154593	3.653427761	20.488801003
4.297542508	2.826082584	22.981200218
5.758496704	3.659039709	20.487198830
-2.881948445	5.320015241	22.985200882
-1.440174990	6.153421037	20.488400459
0.006825678	5.304975415	22.982399464
1.439483745	6.155067202	20.477199554
2.868167375	5.304227036	22.980000973
4.319444649	6.152598177	20.486800671
1.431102925	2.825783322	22.837600708
1.494564507	2.852945054	24.559600353
0.768191236	3.617361972	27.207200527
-0.914900189	4.874729003	27.597999573
0.429672174	5.733275953	27.574400902
1.337228090	2.823763190	25.436799526

2.121187549	2.741080942	27.197999954
5.877038790	4.639253285	26.314799786
-2.993146387	5.740534067	27.383201122
5.189719175	0.093307348	26.307199001
1.999405403	7.402183273	27.356400490
0.053741531	4.847941236	27.838799953
1.204214010	2.748264129	26.848399639
-2.615401320	4.849662329	27.256400585
1.033269625	7.333642842	27.238399982

Pd@Au_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pd H O

26 1 8 4

Cartesian

0.006805336	0.343897199	22.960309982
1.439981225	1.159298866	20.468790531
-0.000043130	1.995370371	17.999999523
2.874126663	0.345005132	22.959573269
4.321913705	1.162968621	20.480182171
2.880047681	1.995370371	17.999999523
5.760391980	0.331865410	22.971868515
7.198681156	1.163182698	20.479969978

5.760052102	1.995370371	17.999999523
-1.426293272	2.825833942	22.959694862
-0.003611754	3.660630795	20.469079018
-1.440045470	4.489527587	17.999999523
2.883877276	3.660276898	20.468561649
1.440045341	4.489527587	17.999999523
4.306105377	2.826470376	22.959761620
5.760177631	3.659496408	20.482971668
4.320049763	4.489527587	17.999999523
-2.879431254	5.321042812	22.975971699
-1.440714828	6.151749449	20.483152866
-2.880047552	6.983684356	17.999999523
0.007207028	5.308881435	22.962055206
1.440003884	6.154052119	20.480129719
0.000043259	6.983684356	17.999999523
2.872846832	5.309335011	22.960376740
4.321143087	6.151735624	20.482130051
2.880047681	6.983684356	17.999999523
1.439586099	2.826615993	22.779626846
1.034667437	3.547374288	27.169027328
-0.693828087	4.919343614	27.629339695
2.362677076	7.238467175	27.335510254
0.657824359	5.751227231	27.616159916
1.472899261	2.800736718	25.861320496
-2.542182045	4.707424432	26.307334900
-2.751500045	5.814014780	27.374448776

5.580026989	0.016308299	26.276557446
0.262588026	4.884475320	27.902462482
1.394824836	7.301409483	27.221713066
1.495603499	2.722469370	26.824216843
-2.404504022	4.910750639	27.251620293

Pd@Au_Rf_top

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pd H O

26 1 9 4

Cartesian

0.003768697	0.336786095	22.951891422
1.440178659	1.170131738	20.471000671
-0.000043130	1.995370371	17.999999523
2.877120284	0.337502195	22.952504158
4.319371907	1.164267914	20.475916862
2.880047681	1.995370371	17.999999523
5.760843433	0.333157345	22.918763161
7.200948915	1.164248179	20.475590229
5.760052102	1.995370371	17.999999523
-1.433791093	2.827060204	22.950003147
0.005134065	3.655495391	20.468504429
-1.440045470	4.489527587	17.999999523

2.875951707	3.655742695	20.468394756
1.440045341	4.489527587	17.999999523
4.313639295	2.827019618	22.951159477
5.760155358	3.655603991	20.478050709
4.320049763	4.489527587	17.999999523
-2.880288986	5.322344224	22.926683426
-1.437131785	6.153753303	20.478003025
-2.880047552	6.983684356	17.999999523
0.002160641	5.314871586	22.953388691
1.440079846	6.151387302	20.476422310
0.000043259	6.983684356	17.999999523
2.877355055	5.315381804	22.953491211
4.317534036	6.153898697	20.477201939
2.880047681	6.983684356	17.999999523
1.440412915	2.828771039	22.846369743
1.441670392	2.861084453	24.416856766
1.030410014	3.555234495	27.288744450
-0.696130865	4.924827116	27.840867043
2.358901169	7.242050294	27.549080849
0.653701092	5.756761131	27.828073502
1.470460268	2.800903520	25.978252888
-2.543509721	4.713129594	26.521015167
-2.752901913	5.818657136	27.587549686
5.576312468	0.020314935	26.492497921
0.262925087	4.884456142	28.103873730
1.393304843	7.307295272	27.438867092

1.491346463	2.731398402	26.950626373
-2.408819864	4.915174904	27.465927601

Pd@Au_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pd H O

26 1 9 4

Cartesian

-0.003790279	0.331844170	22.922518253
1.444495563	1.161748157	20.459761620
-0.000043130	1.995370371	17.999999523
2.870167677	0.282027590	23.000679016
4.319351822	1.165119763	20.472238064
2.880047681	1.995370371	17.999999523
5.777362656	0.322198564	22.926385403
7.199781240	1.166716647	20.469303131
5.760052102	1.995370371	17.999999523
-1.424845796	2.830181719	22.947266102
0.003481075	3.655162010	20.477085114
-1.440045470	4.489527587	17.999999523
2.884452004	3.655686723	20.462162495
1.440045341	4.489527587	17.999999523
4.361326216	2.861383716	23.003861904

5.753687984	3.653049558	20.479922295
4.320049763	4.489527587	17.999999523
-2.858081472	5.308187467	22.959063053
-1.439346113	6.160745604	20.479123592
-2.880047552	6.983684356	17.999999523
0.004904765	5.307141610	22.935776711
1.438345101	6.151217378	20.468862057
0.000043259	6.983684356	17.999999523
2.878352848	5.324321763	22.926888466
4.325478530	6.149034235	20.474033356
2.880047681	6.983684356	17.999999523
1.435845082	2.828270410	22.812111378
2.795986754	2.047095696	23.665535450
2.454047772	2.675810543	26.854517460
0.709084668	4.075163930	27.159657478
3.780476649	6.398294750	26.838381290
2.061118207	4.900429880	27.143905163
2.937882996	1.851736735	25.616230965
-1.137275216	3.865204893	25.784208775
-1.370449198	4.945333050	26.873664856
2.699184458	6.642116363	25.753619671
1.650592849	4.059672757	27.477803230
2.813934286	6.459449067	26.707746983
2.933283684	1.835960015	26.583309174
-1.017031731	4.044321182	26.738862991

Pd@Au_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pd O H

26 1 4 9

Cartesian

0.000296280	0.342584999	22.913637161
1.434348521	1.169359833	20.441114902
-0.000043130	1.995370371	17.999999523
2.865235617	0.345180854	22.873232365
4.320209217	1.163381388	20.445656776
2.880047681	1.995370371	17.999999523
5.755231473	0.324189483	22.901983261
7.198057182	1.161462609	20.454888344
5.760052102	1.995370371	17.999999523
-1.431266676	2.824219442	22.896864414
0.004172449	3.653292179	20.446300507
-1.440045470	4.489527587	17.999999523
2.869293916	3.655686500	20.446805954
1.440045599	4.489527587	17.999999523
4.301378540	2.829103973	22.889719009
5.758096814	3.658174034	20.447201729
4.320049763	4.489527587	17.999999523
-2.889622183	5.316171660	22.903437614

-1.443942400	6.148833092	20.448400974
-2.880047423	6.983684356	17.999999523
0.005106899	5.306411963	22.896533012
1.440088343	6.150204971	20.452160835
0.000043517	6.983684356	17.999999523
2.866950453	5.308306994	22.920699120
4.315442404	6.152033102	20.461044312
2.880047681	6.983684356	17.999999523
1.432619957	2.815568487	22.846317291
-0.691131342	4.191427108	26.825733185
1.548608851	2.861359632	26.230552197
-0.651119446	6.813769380	26.005053520
5.613648538	2.976821581	26.027534008
-0.705043283	5.117922655	26.460356712
-1.506034237	3.746557429	26.465716362
2.270691997	3.515281864	26.180758476
0.706944755	3.399619886	26.392967701
-1.557913949	7.173882714	26.050763130
-0.440252130	6.837944956	25.038621426
1.436596453	2.745983983	24.411613941
5.506803808	3.083379920	25.048813820
5.656906802	2.010291563	26.155619621

Pd@Au_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
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-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Pd H O

26 1 10 4

Cartesian

-0.002281873	0.329496789	22.944400311
1.440459007	1.178052934	20.501563549
-0.000043130	1.995370371	17.999999523
2.882927248	0.330772250	22.944734097
4.320580138	1.163811996	20.472002029
2.880047681	1.995370371	17.999999523
5.759822835	0.331815598	22.949123383
7.200166774	1.163641403	20.472333431
5.760052102	1.995370371	17.999999523
-1.444573375	2.825749872	22.943127155
0.011847733	3.651642668	20.500805378
-1.440045470	4.489527587	17.999999523
2.867897906	3.651163893	20.501947403
1.440045599	4.489527587	17.999999523
4.322812942	2.825752771	22.944481373
5.759922196	3.658872907	20.467920303
4.320049763	4.489527587	17.999999523
-2.879729208	5.320842560	22.949960232
-1.440416649	6.151878788	20.468933582
-2.880047423	6.983684356	17.999999523
-0.001077874	5.325110728	22.946615219

1.440045084	6.152326120	20.472786427
0.000043517	6.983684356	17.999999523
2.881194821	5.324109916	22.944626808
4.320919581	6.152186970	20.468814373
2.880047681	6.983684356	17.999999523
1.436451226	2.826603282	22.924151421
1.440844348	2.841049044	24.637315273
0.730629792	3.683406841	27.230081558
-0.908130516	4.861899080	27.594206333
0.454097380	5.712142059	27.567009926
1.324273129	2.831228468	25.636820793
2.098096296	2.755637979	27.251110077
5.895821250	4.637503648	26.348156929
-2.977562658	5.737995467	27.417657375
5.176846665	0.085123928	26.343512535
1.988680478	7.400620955	27.392714024
0.068241591	4.823259010	27.818179131
1.195173102	2.790763389	26.862857342
-2.581086293	4.856276873	27.284958363
1.026837399	7.298667955	27.265734673

Ni@Au_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Ni H O

26 1 8 4

Cartesian

0.027711937	0.383978750	22.961924076
1.439963136	1.165861341	20.478334427
-0.000043130	1.995370371	17.999999523
2.851194477	0.385550825	22.961587906
4.324573435	1.160946816	20.483436584
2.880047681	1.995370371	17.999999523
5.759417313	0.331868616	22.980120182
7.195483068	1.160929534	20.483317375
5.760052102	1.995370371	17.999999523
-1.380844015	2.825003946	22.962279320
0.001476734	3.657300108	20.478467941
-1.440045470	4.489527587	17.999999523
2.878319503	3.657013111	20.478484631
1.440045341	4.489527587	17.999999523
4.260852942	2.825620757	22.961411476
5.760417745	3.658075246	20.495710373
4.320049763	4.489527587	17.999999523
-2.879381316	5.320432246	22.974560261
-1.440332834	6.151882356	20.496256351
-2.880047552	6.983684356	17.999999523
0.031145569	5.270880475	22.963185310
1.440105595	6.157229830	20.483293533
0.000043259	6.983684356	17.999999523

2.849399850	5.271260462	22.961702347
4.320973912	6.151720014	20.494456291
2.880047681	6.983684356	17.999999523
1.437511719	2.827492372	22.605462074
1.033923534	3.549335326	27.026534081
-0.693461801	4.919165216	27.480897903
2.361002071	7.236382150	27.191772461
0.656672584	5.752390831	27.468411922
1.473145169	2.800126151	25.722403526
-2.539577515	4.710908541	26.158511639
-2.748221361	5.814108884	27.230937481
5.581218788	0.012773152	26.128010750
0.262137152	4.885891352	27.755837440
1.394820716	7.303146186	27.077264786
1.495234123	2.722668506	26.683216095
-2.406175647	4.908664276	27.105436325

Ni@Au_Rf_top

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Ni H O

26 1 9 4

Cartesian

0.019917112	0.369516989	22.930338383
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1.440123620	1.178056279	20.476784706
-0.000043130	1.995370371	17.999999523
2.859595092	0.370566135	22.929444313
4.323183349	1.162543699	20.468473434
2.880047681	1.995370371	17.999999523
5.760492741	0.332171669	22.928731441
7.197780246	1.162066262	20.468389988
5.760052102	1.995370371	17.999999523
-1.396572938	2.823902117	22.928287983
0.011168075	3.652218224	20.474500656
-1.440045470	4.489527587	17.999999523
2.869253231	3.652098920	20.473940372
1.440045341	4.489527587	17.999999523
4.276182394	2.824370634	22.928416729
5.760418003	3.658292446	20.478298664
4.320049763	4.489527587	17.999999523
-2.879988328	5.322080641	22.925035954
-1.438741644	6.152957648	20.478610992
-2.880047552	6.983684356	17.999999523
0.023270598	5.282842047	22.934150696
1.440074181	6.154812539	20.469830036
0.000043259	6.983684356	17.999999523
2.856447746	5.282729210	22.932159901
4.319580349	6.152806456	20.477654934
2.880047681	6.983684356	17.999999523
1.439010855	2.830263336	22.678387165

1.441337837	2.866054839	24.156677723
1.011975816	3.573165034	27.101173401
-0.715370765	4.944949495	27.650766373
2.341336660	7.267452802	27.352333069
0.635858488	5.774357843	27.636835575
1.447795942	2.824070034	25.786967278
-2.567185633	4.729606414	26.332728863
-2.780130467	5.842412140	27.391533852
5.554804498	0.046208352	26.298696995
0.244017484	4.902458263	27.910635471
1.374495603	7.329719429	27.243509293
1.473459570	2.751670189	26.757020950
-2.431494780	4.939571248	27.275876999

Ni@Au_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Ni H O

26 1 9 4

Cartesian

0.017984998	0.367065190	22.916994095
1.449075048	1.160736307	20.464699268
-0.000043130	1.995370371	17.999999523
2.858305090	0.311090012	22.987246513

4.323897704	1.162454389	20.477199554
2.880047681	1.995370371	17.999999523
5.781627885	0.319436827	22.932348251
7.198661522	1.163712651	20.465457439
5.760052102	1.995370371	17.999999523
-1.383472283	2.823361795	22.947607040
0.020390259	3.645814412	20.495181084
-1.440045470	4.489527587	17.999999523
2.887640308	3.651960885	20.467326641
1.440045341	4.489527587	17.999999523
4.329924182	2.857088789	22.992439270
5.763963066	3.652191464	20.483632088
4.320049763	4.489527587	17.999999523
-2.852926421	5.305527556	22.955396175
-1.433170868	6.152195444	20.483045578
-2.880047552	6.983684356	17.999999523
0.032745643	5.274455121	22.940564156
1.440263439	6.153235057	20.465576649
0.000043259	6.983684356	17.999999523
2.859767372	5.288268462	22.921617031
4.328069960	6.147448279	20.481219292
2.880047681	6.983684356	17.999999523
1.470357914	2.808660925	22.629556656
2.660226490	2.125285441	23.562846184
2.454255442	2.674789438	26.824481487
0.707440305	4.076967085	27.130107880

3.780520938	6.402496018	26.800780296
2.058683077	4.903889460	27.115817070
2.946283321	1.846917653	25.590667725
-1.135215513	3.869838330	25.737996101
-1.377237024	4.941761527	26.834182739
2.701570922	6.637231832	25.711176395
1.651053250	4.058575165	27.441897392
2.814208519	6.456278492	26.666369438
2.933946863	1.833757025	26.557247639
-1.013786264	4.045496377	26.693735123

Ni@Au_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Ni O H

26 1 4 9

Cartesian

0.019640482	0.382986134	22.905824184
1.431639866	1.179739128	20.448520184
-0.000043130	1.995370371	17.999999523
2.845068574	0.394066365	22.859921455
4.323895258	1.164167677	20.437335968
2.880047681	1.995370371	17.999999523
5.747650482	0.329181639	22.921195030

7.192150310	1.159714199	20.454597473
5.760052102	1.995370371	17.999999523
-1.386049052	2.825870067	22.885646820
0.006952237	3.654557019	20.452201366
-1.440045470	4.489527587	17.999999523
2.861822440	3.656507130	20.460002422
1.440045599	4.489527587	17.999999523
4.263748345	2.834523475	22.876112461
5.757922232	3.661512749	20.452136993
4.320049763	4.489527587	17.999999523
-2.887134829	5.321183746	22.906186581
-1.445425442	6.152009910	20.454976559
-2.880047423	6.983684356	17.999999523
0.031328133	5.276957596	22.884085178
1.440988545	6.157688758	20.450360775
0.000043517	6.983684356	17.999999523
2.850942502	5.284094845	22.916033268
4.316822835	6.153833582	20.466928482
2.880047681	6.983684356	17.999999523
1.418500474	2.820627848	22.680172920
-0.622968673	4.149628951	26.668939590
1.470186422	2.858618550	25.772452354
-0.636108001	6.804352206	25.993909836
5.628799804	2.972280020	26.008331776
-0.663869828	5.097930953	26.361277103
-1.472317773	3.723808365	26.364881992

2.232271421	3.466977540	25.840115547
0.648104695	3.403761168	26.056480408
-1.556230189	7.133602277	26.010358334
-0.389078598	6.853994068	25.037209988
1.369908716	2.787962990	24.215710163
5.488505567	3.107502200	25.037298203
5.702656460	2.002378729	26.100206375

Ni@Au_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Ni H O

26 1 10 4

Cartesian

-0.000043130	1.995370371	17.999999523
2.880047681	1.995370371	17.999999523
5.760052102	1.995370371	17.999999523
-1.440045470	4.489527587	17.999999523
1.440045341	4.489527587	17.999999523
4.320049763	4.489527587	17.999999523
-2.880047552	6.983684356	17.999999523
0.000043259	6.983684356	17.999999523
2.880047681	6.983684356	17.999999523
0.011525413	0.360789156	22.928290367

1.440188315	1.181719120	20.503907204
2.867882376	0.361873145	22.930757999
4.326268332	1.160845910	20.471651554
5.756743951	0.332672382	22.989997864
7.193587969	1.160791164	20.473237038
-1.412334595	2.824916308	22.936248779
0.014397320	3.651181956	20.507481098
2.865787091	3.649969297	20.505328178
4.291375760	2.825056351	22.931253910
5.761056590	3.661492010	20.472140312
-2.878718668	5.320266336	22.967660427
-1.441190550	6.150598338	20.474765301
0.017417736	5.298630698	22.943432331
1.440060791	6.158648984	20.474872589
2.864470261	5.301101507	22.930581570
4.324287101	6.150776735	20.473423004
1.427821022	2.832129154	22.727575302
1.506246670	2.819912696	24.358136654
0.881127784	3.737403169	27.006654739
-0.796852622	4.987558915	27.383496761
0.541717275	5.851828867	27.358939648
1.392393182	2.871184221	25.230801105
2.240053693	2.870688276	26.966543198
-2.627463900	4.778793361	26.056292057
-2.874169455	5.842082104	27.160441875
5.339794333	0.177063598	26.042299271

6.433248973	0.017840124	27.132096291
0.168160993	4.970162455	27.637836933
1.310139999	2.862505169	26.654980183
-2.491926257	4.956892781	27.007431984
1.149985171	7.444684317	26.987438202

Cu@Au_Rf_sur

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Cu H O
26 1 8 4

Cartesian

0.021394345	0.373669281	22.934107780
1.440033496	1.165990791	20.481271744
-0.000043130	1.995370371	17.999999523
2.858280483	0.374773368	22.934486866
4.325099305	1.161062663	20.477075577
2.880047681	1.995370371	17.999999523
5.760155293	0.330513685	22.974431515
7.195138797	1.161482121	20.477089882
5.760052102	1.995370371	17.999999523
-1.393026475	2.824195804	22.934889793
0.002306640	3.657453976	20.482926369
-1.440045470	4.489527587	17.999999523

2.878183545	3.657278923	20.481772423
1.440045341	4.489527587	17.999999523
4.273155283	2.824262703	22.935092449
5.760061630	3.659841830	20.476605892
4.320049763	4.489527587	17.999999523
-2.878494406	5.319195949	22.937152386
-1.440768130	6.151431455	20.477247238
-2.880047552	6.983684356	17.999999523
0.025714999	5.281928650	22.940254211
1.439973758	6.157484938	20.477497578
0.000043259	6.983684356	17.999999523
2.854891446	5.281492914	22.935907841
4.321634130	6.151530912	20.476942062
2.880047681	6.983684356	17.999999523
1.440721909	2.825361857	22.651164532
1.035011064	3.545371550	27.018735409
-0.691862499	4.918325409	27.484681606
2.363131812	7.243576487	27.179934978
0.659372935	5.746724917	27.470378876
1.474184419	2.799659641	25.712757111
-2.543447778	4.709187449	26.151421070
-2.758819857	5.814214139	27.219076157
5.584504836	0.014795470	26.115052700
0.262483998	4.883539178	27.763457298
1.395873356	7.307496416	27.063875198
1.496864839	2.720983985	26.674022675

-2.409930955 4.910833594 27.096750736

Cu@Au_Rf_top

1.0

8.6400995255 0.0000000000 0.0000000000
-4.3200497627 7.4825456803 0.0000000000
0.0000000000 0.0000000000 40.0000000000

Au Cu H O

26 1 9 4

Cartesian

0.007613082 0.347019662 22.926754951
1.440301227 1.174785690 20.492186546
-0.000043130 1.995370371 17.999999523
2.872442581 0.346341443 22.927393913
4.321970869 1.162785763 20.472116470
2.880047681 1.995370371 17.999999523
5.760058475 0.329665403 22.944169044
7.198082738 1.162500326 20.471684933
5.760052102 1.995370371 17.999999523
-1.420393320 2.821699127 22.925765514
0.008391377 3.653335217 20.489323139
-1.440045470 4.489527587 17.999999523
2.871588325 3.653758689 20.488502979
1.440045341 4.489527587 17.999999523
4.300045489 2.821898041 22.926800251
5.759870954 3.658419331 20.470774174

4.320049763	4.489527587	17.999999523
-2.880154396	5.318779390	22.919239998
-1.439762225	6.151921157	20.470890999
-2.880047552	6.983684356	17.999999523
0.011967339	5.301042190	22.931747437
1.439794026	6.153855435	20.473892689
0.000043259	6.983684356	17.999999523
2.868288655	5.301927935	22.931253910
4.319704204	6.152131667	20.471291542
2.880047681	6.983684356	17.999999523
1.442752515	2.822352286	22.700982094
1.446299896	2.887703634	24.220650196
1.012793491	3.586062079	27.109625340
-0.714113160	4.957107305	27.666742802
2.340137764	7.272543383	27.377386093
0.633886334	5.789055591	27.654249668
1.452221895	2.834600186	25.793023109
-2.561261155	4.745453935	26.347808838
-2.768810020	5.850236667	27.416357994
5.558895545	0.050755771	26.317541599
0.244044521	4.917309879	27.932598591
1.373647415	7.338311066	27.263405323
1.471982321	2.764222258	26.768445969
-2.426153721	4.945624285	27.292444706

Cu@Au_Rf_fcc

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Cu H O

26 1 9 4

Cartesian

0.007040719	0.371887812	22.908346653
1.445672831	1.167519548	20.469977856
-0.000043130	1.995370371	17.999999523
2.843872831	0.292572628	23.001546860
4.317613216	1.166081328	20.467817783
2.880047681	1.995370371	17.999999523
5.764331959	0.328615365	22.920649052
7.195096439	1.165901257	20.460879803
5.760052102	1.995370371	17.999999523
-1.396764434	2.824670342	22.933456898
0.013810231	3.650342148	20.493733883
-1.440045470	4.489527587	17.999999523
2.880352297	3.651735881	20.472006798
1.440045341	4.489527587	17.999999523
4.338702574	2.878391492	23.004388809
5.753833726	3.654474956	20.477006435
4.320049763	4.489527587	17.999999523
-2.873883459	5.317313852	22.926981449
-1.439608243	6.160053867	20.478239059

-2.880047552	6.983684356	17.999999523
0.024375767	5.283359847	22.931282520
1.435729467	6.154805850	20.463044643
0.000043259	6.983684356	17.999999523
2.849515207	5.295102435	22.913641930
4.321688204	6.151562132	20.466105938
2.880047681	6.983684356	17.999999523
1.445732119	2.822201317	22.694146633
2.840696518	2.020305477	23.627855778
2.451459818	2.678344014	26.846046448
0.710755553	4.075015859	27.154731750
3.784461127	6.395078238	26.840376854
2.066512986	4.896336989	27.137346268
2.950392426	1.850965053	25.611820221
-1.155914959	3.850324734	25.806410313
-1.369455396	4.951232665	26.878767014
2.690387655	6.666820443	25.775165558
1.655693568	4.052093527	27.462711334
2.818024852	6.446488468	26.719298363
2.928257703	1.836008963	26.581361294
-1.008355436	4.054030035	26.752083302

Cu@Au_Volmer

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000

0.0000000000 0.0000000000 40.0000000000

Au Cu O H

26 1 4 9

Cartesian

0.011990530	0.368695467	22.905352116
1.432257726	1.176235841	20.451016426
-0.000043130	1.995370371	17.999999523
2.855334161	0.379362317	22.855925560
4.322721016	1.164388109	20.435159206
2.880047681	1.995370371	17.999999523
5.752717517	0.332981428	22.912828922
7.195149290	1.160091176	20.451707840
5.760052102	1.995370371	17.999999523
-1.404331907	2.827207382	22.880444527
0.008527205	3.651781149	20.459334850
-1.440045470	4.489527587	17.999999523
2.860771989	3.653916571	20.469849110
1.440045599	4.489527587	17.999999523
4.282868253	2.833929634	22.868592739
5.758665491	3.659551042	20.445520878
4.320049763	4.489527587	17.999999523
-2.884092799	5.323885135	22.881810665
-1.444941738	6.151724028	20.446498394
-2.880047423	6.983684356	17.999999523
0.021299217	5.296224557	22.870423794
1.441133515	6.155754480	20.444962978

0.000043517	6.983684356	17.999999523
2.861724592	5.305093603	22.900490761
4.316138928	6.154044983	20.458557606
2.880047681	6.983684356	17.999999523
1.419728597	2.813214305	22.714767456
-0.659591162	4.174659054	26.712741852
1.510408176	2.847742529	25.977468491
-0.638955639	6.819326025	25.982186794
5.616939067	2.967634541	25.994727612
-0.687188063	5.112762945	26.377420425
-1.491090706	3.738173179	26.380176544
2.248321215	3.486148389	25.947701931
0.681955378	3.397137035	26.194350719
-1.555065539	7.159512772	26.001660824
-0.396839755	6.858303712	25.024037361
1.374105370	2.694394687	24.263417721
5.488796536	3.093328496	25.021092892
5.686593662	1.998460667	26.097445488

Cu@Au_Heyrovsky

1.0

8.6400995255	0.0000000000	0.0000000000
-4.3200497627	7.4825456803	0.0000000000
0.0000000000	0.0000000000	40.0000000000

Au Cu H O

26 1 10 4

Cartesian

-0.001499571	0.350294627	22.919061184
1.436550619	1.179994348	20.521030426
-0.000043130	1.995370371	17.999999523
2.871940369	0.349489440	22.920019627
4.321199800	1.161836910	20.467228889
2.880047681	1.995370371	17.999999523
5.751207969	0.328373608	22.996873856
7.190476657	1.161468630	20.468842983
5.760052102	1.995370371	17.999999523
-1.434063571	2.826071880	22.924075127
0.009518175	3.652295158	20.524990559
-1.440045341	4.489527587	17.999999523
2.862333439	3.651253092	20.523927212
1.440045599	4.489527587	17.999999523
4.307967452	2.823290658	22.912247181
5.757214507	3.664427992	20.453319550
4.320049763	4.489527587	17.999999523
-2.886107826	5.317435609	22.962009907
-1.448397321	6.149728648	20.457084179
-2.880047423	6.983684356	17.999999523
0.003396359	5.318382455	22.928307056
1.435657368	6.156845828	20.466234684
0.000043517	6.983684356	17.999999523
2.866845138	5.323623782	22.913005352
4.322906670	6.149769234	20.456593037

2.880047681	6.983684356	17.999999523
1.406487044	2.811864503	22.778513432
1.625163154	2.960031004	24.397485256
0.701313210	3.684704685	26.904220581
-0.942987747	4.882813991	27.060086727
0.401923222	5.739238007	27.033965588
1.374042927	2.870878938	25.306322575
2.035894380	2.737590590	26.999428272
-2.590258652	4.851800873	25.511157513
-3.060202921	5.572510554	26.810984612
1.075579406	7.269533366	25.471990108
1.897566376	7.455552311	26.785080433
0.000149605	4.897649105	27.396960258
1.148408013	2.783244145	26.578452587
-2.559920572	4.795940064	26.495020390
1.002975592	7.245079489	26.455779076