

Electronic Supplementary Information for:

How covalence breaks adsorption-energy scaling relations and solvation restores them

Federico Calle-Vallejo,^{1,*} Alexander Krabbe,² Juan María García-Lastra^{2,*}

¹ Leiden Institute of Chemistry, Leiden University, P. O. Box 9502, 2300 RA Leiden, The Netherlands.

² Department of Energy Conversion & Storage, Technical University of Denmark, DK-4000 Roskilde, Denmark.

*Emails: f.calle.vallejo@chem.leidenuniv.nl, jmgla@dtu.dk

Table of contents

S1. Assessment of adsorption energies	2
S2. Modelling the oxygen evolution and reduction reactions	6
S3. Details of the calculations in ADF	7
S4. Spin states	9
S.5. References	11
S.6. Cartesian coordinates of the systems under study	12

S1. Assessment of adsorption energies

The free energies in vacuum were estimated from DFT energies in the following way: $G^{vac} = E_{DFT} + ZPE - TS$. The zero-point energies (ZPE) of the molecules appear in Table S1 and were taken from previous studies.¹⁻⁴ Entropic corrections (TS) for molecules were also taken from those studies and correspond to $T = 298.15$ K. The free energies in solution contain an additional solvation term: $G^{solv} = E_{DFT} + ZPE - TS + E_{solv}$. E_{solv} is calculated using the COSMO approach.⁵

Moreover, Table S2 contains the ZPE corrections for the porphyrins under study, Table S3 contains their solvation energies (see details of those calculations in section S4), and Table S4 contains the DFT adsorption energies without any corrections.

Table S1. ZPE and entropic corrections at 298.15 K in eV for the molecules in this study, from¹⁻⁴.

correction / species	H ₂ O	H ₂
TS	0.67	0.41
ZPE	0.56	0.27

Table S2. ZPE in eV for the porphyrins (with and without adsorbates) in this study.

transition metal	ligand	clean	*O	*OH	*OOH
Cr	H	7.193	7.297	7.530	7.631
	F	4.588	4.692	4.921	5.025
	OH	8.536	8.643	8.870	8.969
	CH ₃	15.996	16.086	16.327	16.413
	BH ₂	10.947	11.058	11.284	11.378
	NH ₂	12.604	12.702	12.934	13.032
Mn	H	7.185	7.278	7.494	7.606
	F	4.585	4.665	4.872	4.998
	OH	8.531	8.617	8.831	8.945
	CH ₃	15.975	16.073	16.300	16.393
	BH ₂	10.904	11.032	11.255	11.358
	NH ₂	12.552	12.674	12.896	12.997
Fe	H	7.211	7.297	7.504	7.599
	F	4.606	4.686	4.868	5.001
	OH	8.560	8.638	8.848	8.948
	CH ₃	15.993	16.088	16.308	16.418
	BH ₂	10.938	11.054	11.273	11.381
	NH ₂	12.584	12.693	12.872	12.982
Co	H	7.223	7.249	7.552	7.624
	F	4.616	4.638	4.952	5.060
	OH	8.568	8.583	8.897	9.005
	CH ₃	16.015	16.056	16.357	16.455
	BH ₂	10.954	11.015	11.323	11.429
	NH ₂	12.613	12.627	12.950	13.052
Ni	H	7.225	7.234	7.518	7.626
	F	4.613	4.621	4.888	4.990
	OH	8.559	8.554	8.848	8.952
	CH ₃	16.021	16.024	16.327	16.309
	BH ₂	10.989	10.987	11.285	11.305
	NH ₂	12.605	12.596	12.883	12.981
Cu	H	7.180	7.198	7.470	7.582
	F	4.561	4.573	4.844	4.949
	OH	8.515	8.509	8.792	8.922
	CH ₃	15.978	15.982	16.256	16.364
	BH ₂	10.904	10.937	11.217	11.340
	NH ₂	12.566	12.542	12.812	12.946

Table S3. Solvation energies in eV for the porphyrins (with and without adsorbates) in this study.

transition metal	ligand	clean	*O	*OH	*OOH
Cr	H	-0.603	-0.887	-0.967	-0.982
	F	-0.271	-0.432	-0.554	-0.564
	OH	-1.398	-1.665	-1.756	-1.730
	CH ₃	-0.757	-1.039	-1.055	-1.142
	BH ₂	-0.263	-0.432	-0.540	-0.574
	NH ₂	-1.626	-1.971	-2.039	-2.063
Mn	H	-0.597	-1.179	-1.120	-1.145
	F	-0.279	-0.674	-0.567	-0.623
	OH	-1.377	-1.977	-1.746	-1.790
	CH ₃	-0.752	-1.333	-1.214	-1.282
	BH ₂	-0.277	-0.718	-0.588	-0.650
	NH ₂	-1.624	-2.401	-2.229	-2.284
Fe	H	-0.613	-1.027	-0.951	-0.931
	F	-0.270	-0.546	-0.467	-0.504
	OH	-1.380	-1.817	-1.753	-1.802
	CH ₃	-0.806	-1.176	-1.110	-1.118
	BH ₂	-0.253	-0.579	-0.543	-0.544
	NH ₂	-1.654	-2.213	-2.075	-2.094
Co	H	-0.608	-1.012	-0.944	-0.935
	F	-0.255	-0.536	-0.552	-0.489
	OH	-1.371	-1.813	-1.757	-1.705
	CH ₃	-0.777	-1.176	-1.057	-1.024
	BH ₂	-0.250	-0.512	-0.556	-0.492
	NH ₂	-1.683	-2.390	-2.128	-2.076
Ni	H	-0.659	-0.824	-1.152	-0.980
	F	-0.239	-0.404	-0.613	-0.422
	OH	-1.426	-1.757	-1.914	-1.717
	CH ₃	-0.820	-1.009	-1.164	-1.195
	BH ₂	-0.248	-0.389	-0.663	-0.560
	NH ₂	-1.736	-2.297	-2.361	-2.260
Cu	H	-0.627	-1.057	-1.109	-0.732
	F	-0.246	-0.610	-0.676	-0.454
	OH	-1.385	-1.878	-1.824	-1.559
	CH ₃	-0.792	-1.558	-1.474	-0.966
	BH ₂	-0.244	-0.558	-0.631	-0.518
	NH ₂	-1.684	-2.804	-2.704	-2.126

Table S4. DFT energies of adsorption (ΔE) in eV for the porphyrins (with and without adsorbates) in this study.

transition metal	ligand	*O	*OH	*OOH
Cr	H	1.05	0.25	3.45
	F	1.09	0.29	3.47
	OH	0.95	0.20	3.38
	CH ₃	0.83	0.11	3.29
	BH ₂	1.02	0.25	3.45
	NH ₂	0.88	0.14	3.32
Mn	H	1.45	0.44	3.64
	F	1.47	0.42	3.62
	OH	1.28	0.25	3.50
	CH ₃	1.25	0.28	3.49
	BH ₂	1.75	0.67	3.85
	NH ₂	1.14	0.17	3.38
Fe	H	1.54	0.63	3.69
	F	1.59	0.57	3.68
	OH	1.46	0.52	3.64
	CH ₃	1.40	0.52	3.60
	BH ₂	1.75	0.79	3.92
	NH ₂	1.38	0.43	3.47
Co	H	2.71	1.18	4.00
	F	2.25	0.96	3.86
	OH	2.11	0.90	3.84
	CH ₃	2.53	0.90	3.86
	BH ₂	2.70	1.13	4.04
	NH ₂	1.98	0.84	3.80
Ni	H	3.84	1.98	4.75
	F	3.61	1.91	4.72
	OH	3.58	1.74	4.67
	CH ₃	4.03	1.84	4.67
	BH ₂	4.02	2.01	4.77
	NH ₂	3.70	1.62	4.59
Cu	H	4.56	2.22	4.76
	F	4.53	2.15	4.82
	OH	4.22	1.96	4.69
	CH ₃	4.55	2.20	4.66
	BH ₂	4.95	2.39	4.81
	NH ₂	3.87	1.65	4.53

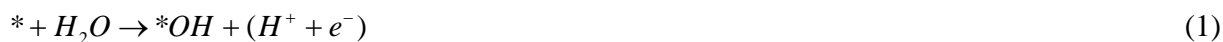
The effects of -F, -OH, CH₃ and -NH₂ and -BH₂ on the binding energies of *OH on centers with metals from Cr to Cu are presented in Table S5, with respect to conventional porphyrin rings with -H ligands. The table contains differences in the adsorption energies, so that the value of -0.27 eV for Co rings with -CH₃ ligands means that, compared to a ring with -H ligands, the *OH adsorption energies are strengthened by 0.27 eV.

Table S5. Ligand effects on the adsorption energies of *OH on porphyrins with metal centers from Cr to Cu. All values are in eV and represent the adsorption energies with respect to those of the corresponding rings with -H ligands.

metal/ligand	-F	-OH	-CH ₃	-BH ₂	-NH ₂
Cr	0.04	-0.05	-0.14	0.01	-0.11
Mn	-0.02	-0.19	-0.16	0.22	-0.27
Fe	-0.06	-0.11	-0.11	0.16	-0.20
Co	-0.22	-0.28	-0.27	-0.04	-0.34
Ni	-0.07	-0.24	-0.14	0.03	-0.36
Cu	-0.08	-0.26	-0.02	0.16	-0.58

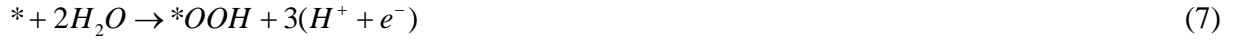
S2. Modelling the oxygen evolution and reduction reactions

We used the computational hydrogen (CHE) approach⁶ to model concerted proton-electron transfers. In it, the energetics of H₂(g) is used instead of that of (H⁺+e⁻) as an electrochemical reference due to the following relationship in equilibrium: $\mu(H^+ + e^-) = \frac{1}{2}\mu(H_2)$. In previous studies we used the following OER mechanism^{3,4}:



Here * denotes a free adsorption site at the metal center of a porphyrin ring. The adsorption energies of *O, *OH and *OOH are calculated using the following reactions:





Note that the free energies of reactions (5-7) are ΔG_O , ΔG_{OH} , ΔG_{OOH} , respectively and can be assessed in vacuum and in solution. It can be shown that the free energies of reactions (1-4) can be represented in terms of those of reactions (5-7) as follows,⁷ with $\Delta G_{O_2} = 1.23 \text{ V} \times 4e^- = 4.92 \text{ eV}$:

$$\Delta G_1 = \Delta G_{OH} \quad (8)$$

$$\Delta G_2 = \Delta G_O - \Delta G_{OH} \quad (9)$$

$$\Delta G_3 = \Delta G_{OOH} - \Delta G_O \quad (10)$$

$$\Delta G_4 = \Delta G_{O_2} - \Delta G_{OOH} \quad (11)$$

Finally, the OER overpotential is estimated as the maximal free energy among those in the reaction pathway (1-4) and the corresponding reaction is known as the potential determining step (PDS). Typically, reactions (2) and (3) are potential-limiting for the OER.

$$\eta_{OER} = \max(\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4) - 1.23 \quad (12)$$

The mechanism of the ORR is the inverse of reactions (1-4), and the typical PDSs are reactions (1) and (4). The overpotential is in this case defined as follows:

$$\eta_{ORR} = 1.23 - \min(\Delta G_1, \Delta G_2, \Delta G_3, \Delta G_4) \quad (13)$$

S3. Details of the calculations in ADF

Solvation energies, Bader charges, and zero-phonon energies were computed using the Amsterdam Density Functional (ADF) package, v. 2013.⁸ In all these calculations the geometry was kept frozen to the relaxed geometry found in the VASP calculations. For the sake of consistency with the VASP calculations the RPBE exchange-correlation functional was employed. All atoms were described through basis sets of TZP quality (triple- ζ STO plus one polarization function) given in the program database, including all the core electrons in the calculation (i.e. with no frozen core approximation).

Solvation energies were calculated using the Conductor like Screening Model (COSMO)⁵ as implemented in ADF. The solvation energy was computed as the difference in total energy between a calculation without any solvent (gas phase) and a calculation in which water was modelled as the solvent (we took 78.39 as the relative dielectric constant and 1.93 as the radius of the rigid sphere solvent molecules). The Bader analysis was carried out using the default parameters of the code.⁹ The zero-phonon energies were calculated employing the analytical second derivatives.

Finally, it is important to verify that the presence of explicit water will not change the main conclusions of this study. Thus, we added 3 explicit water molecules around *OH and *OOH as shown below in Fig. S1. The solvation energies of *OH and *OOH with 3 explicit water molecules were calculated on the rings with -H and -F ligands and all metal centers and the comparison with respect to the case in which water is only implicit is given in Fig. S2. Ideally, if the implicit method describes well the adsorbate-solvent interactions, all points should fall on the red dashed line. According to Fig. S2, there is a good agreement between the solvation energy differences calculated with implicit and explicit water.

In practical terms, such good agreement between explicit and implicit solvation shows that the use of an implicit method to account for solvent-adsorbate interactions is suitable in the particular case of porphyrin rings. This is a useful conclusion, as implicit solvation methods are substantially more affordable in computational terms compared to the explicit ones.

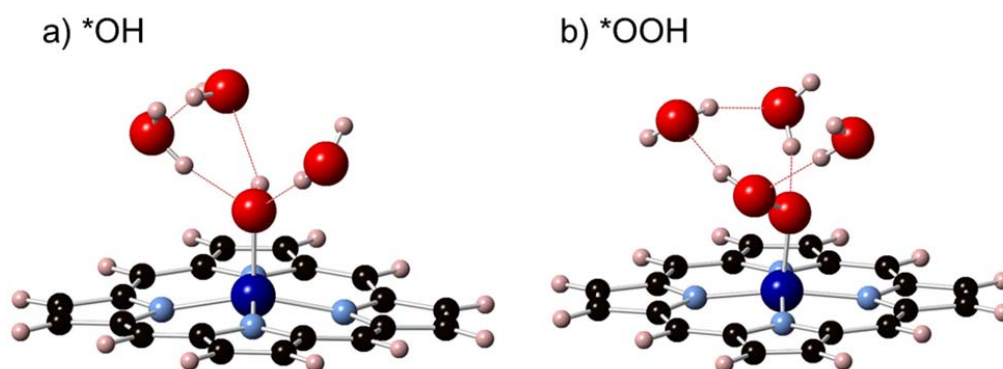


Fig. S1 Three explicit water molecules in the first solvation shell of a) *OH and b) *OOH.

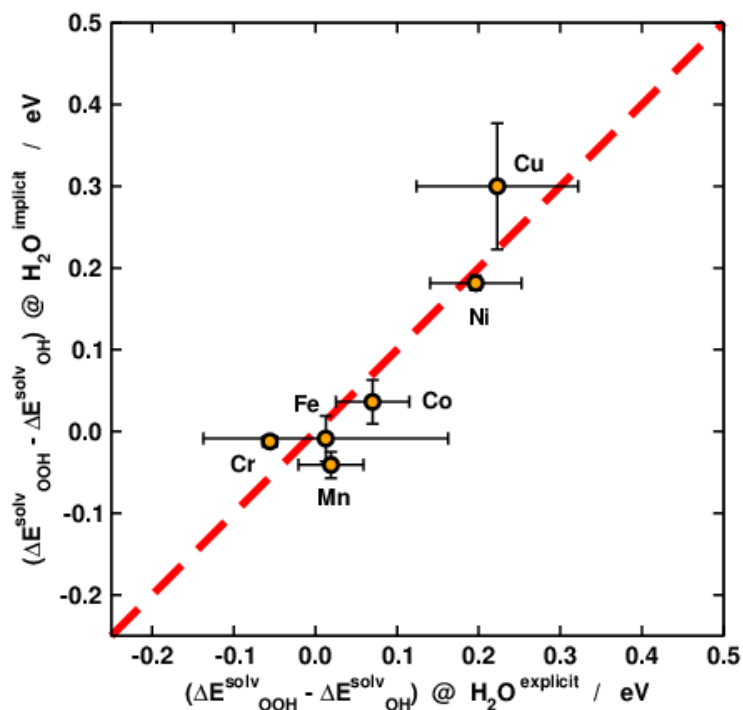


Fig. S2 Comparison between the differences in *OOH and *OH solvation with “explicit” and “implicit” water. “Implicit” water is modelled with COSMO, while “explicit” water is a combination of a first shell of 3 explicit water molecules plus COSMO in the surroundings.

S4. Spin states

In Table S6 we provide the ground-state spin configuration, namely the difference between the number of electrons with spin up minus the number of electrons with spin down, for all the systems considered in this study. In each case, several spin values were considered, so that Table S6 contains only the most stable ones. The values are commensurate with those of previous studies.^{3, 4, 10}

Table S6. Ground-state spin configuration (i.e. number of electrons with spin up minus number of electrons with spin down) for all the systems considered in this study.

Transition Metal	ligand	clean	*O	*OH	*OOH
Cr	H	4	0	3	3
	F	4	0	3	3
	OH	4	0	3	3
	CH ₃	4	0	3	3
	BH ₂	4	0	3	3
	NH ₂	4	0	3	3
Mn	H	3	3	4	4
	F	3	3	4	4
	OH	3	3	4	4
	CH ₃	3	3	4	4
	BH ₂	3	3	4	4
	NH ₂	3	3	4	4
Fe	H	2	2	3	1
	F	2	2	5	3
	OH	2	2	5	1
	CH ₃	2	2	3	1
	BH ₂	2	2	3	3
	NH ₂	2	2	3	1
Co	H	1	3	2	0
	F	1	3	0	0
	OH	1	3	0	0
	CH ₃	1	3	0	0
	BH ₂	1	3	0	0
	NH ₂	1	3	0	0
Ni	H	0	4	1	1
	F	0	4	1	3
	OH	0	4	1	1
	CH ₃	0	4	1	1
	BH ₂	0	4	1	1
	NH ₂	0	4	1	1
Cu	H	1	3	2	2
	F	1	3	2	2
	OH	1	3	2	2
	CH ₃	1	3	2	2
	BH ₂	1	3	2	2
	NH ₂	1	1	0	2

S.5. References

1. I. C. Man, H.-Y. Su, F. Calle-Vallejo, H. A. Hansen, J. I. Martínez, N. G. Inoglu, J. Kitchin, T. F. Jaramillo, J. K. Nørskov and J. Rossmeisl, *ChemCatChem*, 2011, **3**, 1159-1165.
2. J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. R. Kitchin, T. Bligaard and H. Jónsson, *The Journal of Physical Chemistry B*, 2004, **108**, 17886-17892.
3. F. Calle-Vallejo, J. Ignacio Martinez and J. Rossmeisl, *Physical Chemistry Chemical Physics*, 2011, **13**, 15639-15643.
4. F. Calle-Vallejo, J. I. Martinez, J. M. Garcia-Lastra, E. Abad and M. T. M. Koper, *Surface Science*, 2013, **607**, 47-53.
5. A. Klamt and G. Schuurmann, *Journal of the Chemical Society, Perkin Transactions 2*, 1993, 799-805.
6. J. K. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. R. Kitchin, T. Bligaard and H. Jónsson, *Journal of Physical Chemistry B*, 2004, **108**, 17886-17892.
7. F. Calle-Vallejo and M. T. M. Koper, *Electrochimica Acta*, 2012, **84**, 3-11.
8. G. te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. van Gisbergen, J. G. Snijders and T. Ziegler, *Journal of Computational Chemistry*, 2001, **22**, 931-967.
9. J. I. Rodríguez, R. F. W. Bader, P. W. Ayers, C. Michel, A. W. Götz and C. Bo, *Chemical Physics Letters*, 2009, **472**, 149-152.
10. M. T. de Groot and M. T. M. Koper, *Physical Chemistry Chemical Physics*, 2008, **10**, 1023-1031.

S.6. Cartesian coordinates of the systems under study

In the following pages the cartesian coordinates of all the systems included in this study are listed. Firstly we list all the systems used in the calculations where the first solvation shell was not explicitly included. Secondly we list the cartesian coordinates of the systems which include the first solvation shell detailed in Fig. S1.

Systems with no explicit solvation

Transition Metal: Co; Functional Group: BH2; Adsorbate: Clean

H	8.335170000000000	16.543959999999998	6.071920000000000
H	10.000249999999999	17.597760000000001	6.701530000000000
H	6.251020000000000	13.820700000000000	8.417420000000000
H	6.803050000000000	15.420260000000001	7.353760000000000
H	11.712899999999999	4.398790000000000	6.785060000000000
H	13.341360000000000	5.434300000000000	6.040480000000000
H	14.856790000000000	6.586960000000000	7.289320000000000
H	15.620930000000000	8.255160000000000	6.448620000000000
H	9.005060000000000	4.890110000000000	8.173260000000001
H	8.664990000000000	5.238420000000000	6.169350000000000
H	13.711620000000000	15.574490000000001	6.178350000000000
H	12.912080000000000	17.285480000000000	6.926110000000000
H	6.241170000000000	7.695710000000000	7.687740000000000
H	7.689950000000000	6.267910000000000	7.650840000000000
H	16.385320000000000	13.469860000000001	8.629970000000000
H	17.450250000000000	11.894510000000000	7.813680000000000
H	15.451230000000001	8.165550000000000	8.365970000000001
H	17.141749999999998	8.974690000000001	7.584700000000000
H	13.639060000000001	15.788110000000000	8.091049999999999
H	15.289009999999999	14.986170000000000	7.258220000000000
H	4.558410000000000	12.995080000000000	7.642680000000000
H	6.070110000000000	13.745870000000000	6.500420000000000
H	4.886040000000000	8.916190000000000	6.704730000000000
H	5.022670000000000	8.977169999999999	8.764279999999999
C	10.154230000000000	15.262670000000000	7.011730000000000
C	9.685240000000000	13.871740000000001	7.158060000000000
C	8.351070000000000	13.426420000000000	7.274070000000000
C	11.578390000000001	6.732250000000000	7.068460000000000
C	12.035510000000000	8.133860000000000	7.157970000000000
C	13.345879999999999	8.600770000000001	7.238740000000000
C	10.189970000000001	6.777080000000000	7.236120000000000
C	9.844500000000000	8.178500000000000	7.342320000000000
C	11.550150000000000	15.180920000000000	7.101620000000000
C	8.492830000000000	8.557079999999999	7.480330000000000
C	15.104300000000000	11.714359999999999	7.581180000000000
C	11.887130000000001	13.795740000000000	7.240210000000000
C	13.708500000000001	12.179550000000001	7.465260000000000
C	15.026770000000001	10.323480000000000	7.469960000000000
C	13.633170000000000	9.979730000000000	7.356510000000000
C	13.257199999999999	13.497610000000000	7.353220000000000
C	6.686720000000000	11.670859999999999	7.517230000000000
C	8.077700000000000	12.066670000000000	7.394840000000000
C	6.672320000000000	10.284440000000000	7.578170000000000
C	8.085330000000001	9.899670000000000	7.492250000000000
B	9.420560000000000	16.548249999999999	6.584490000000000
B	6.969070000000000	14.238020000000001	7.363750000000000
B	12.288910000000000	5.445640000000000	6.617570000000000
B	14.712280000000000	7.771150000000000	7.312490000000000
B	9.097670000000001	5.635720000000000	7.226240000000000
B	12.829110000000000	16.098800000000001	7.053080000000000
B	7.456850000000000	7.486270000000000	7.593990000000000
B	16.394580000000001	12.436340000000000	8.018969999999999
B	15.951990000000000	9.050870000000000	7.486440000000000
B	14.101739999999999	14.856790000000000	7.244030000000000
B	5.749330000000000	12.927659999999999	7.535190000000000
B	5.517620000000000	9.220560000000001	7.689040000000000
Co	10.866970000000000	11.019560000000000	7.329580000000000
N	10.765359999999999	12.989520000000001	7.262910000000000
N	10.938490000000000	9.005810000000000	7.282540000000000
N	12.825630000000000	11.092129999999999	7.364000000000000
N	8.930280000000000	10.975199999999999	7.390650000000000

Transition Metal: Co; Functional Group: BH2; Adsorbate: O

C	10.153540000000000	15.293860000000000	6.646900000000000
C	9.679779999999999	13.900869999999999	6.806140000000000
C	8.349330000000000	13.437130000000000	6.932910000000000
C	11.574930000000000	6.696610000000000	6.713740000000000
C	12.032140000000000	8.102169999999999	6.822270000000000
C	13.336280000000000	8.593810000000000	6.903970000000000
C	10.186909999999999	6.740240000000000	6.897430000000000
C	9.845549999999999	8.147449999999999	7.032390000000000
C	11.549239999999999	15.209050000000000	6.744730000000000
C	8.499450000000000	8.548970000000001	7.193350000000000
C	15.099890000000000	11.718959999999999	7.210160000000000
C	11.880440000000000	13.820910000000000	6.901100000000000
C	13.701580000000000	12.189740000000000	7.158420000000000
C	15.014670000000001	10.328279999999999	7.092600000000000
C	13.617509999999999	9.978920000000000	7.038250000000000
C	13.247529999999999	13.510320000000000	7.038210000000000
C	6.697380000000000	11.668609999999999	7.167660000000000
C	8.086940000000000	12.076350000000000	7.091890000000000
C	6.688580000000000	10.280200000000001	7.231930000000000
C	8.105510000000001	9.899910000000000	7.207520000000000
B	9.422630000000000	16.583850000000002	6.222660000000000
B	6.954730000000000	14.233879999999999	6.959450000000000
B	12.283740000000000	5.407720000000000	6.264100000000000
B	14.713260000000000	7.777040000000000	6.916420000000000
B	9.094709999999999	5.601620000000000	6.890920000000000
B	12.836020000000000	16.117960000000000	6.712410000000000
B	7.442950000000000	7.499150000000000	7.291000000000000
B	16.418859999999999	12.431870000000000	7.578620000000000
B	15.947960000000000	9.060620000000000	7.052490000000000
B	14.097849999999999	14.870160000000000	6.932720000000000
B	5.745930000000000	12.916150000000000	7.117210000000000
B	5.542070000000000	9.198090000000001	7.259450000000000
Co	10.869510000000000	11.041340000000000	7.358810000000000
H	8.339710000000000	16.583549999999999	5.706200000000000
H	10.002440000000000	17.631489999999999	6.352630000000000
H	6.204990000000000	13.835710000000001	7.996280000000000
H	6.778460000000000	15.413470000000000	6.910740000000000
H	11.692909999999999	4.366050000000000	6.411540000000000
H	13.350099999999999	5.387720000000000	5.714560000000000
H	14.863460000000000	6.594750000000000	6.871010000000000
H	15.582689999999999	8.276020000000001	6.020630000000000
H	8.987190000000000	4.873600000000000	7.848770000000000
H	8.647470000000000	5.208630000000000	5.840010000000000
H	13.728899999999999	15.581280000000000	5.856010000000000
H	12.932010000000000	17.303300000000000	6.582250000000000
H	6.226890000000000	7.730910000000000	7.399040000000000
H	7.654050000000000	6.278870000000000	7.318300000000000
H	16.454560000000001	13.475090000000000	8.169729999999999
H	17.454219999999999	11.867250000000000	7.335750000000000
H	15.490580000000000	8.164360000000000	7.943580000000000
H	17.141150000000000	8.995279999999999	7.101490000000000
H	13.621779999999999	15.804720000000000	7.767820000000000
H	15.283700000000000	14.999230000000001	6.971090000000000
H	4.551380000000000	12.969300000000000	7.180320000000000
H	6.092710000000000	13.712500000000000	6.075190000000000
H	5.003740000000000	8.884090000000000	6.223320000000000
H	4.928660000000000	9.001700000000000	8.282260000000001
O	10.901719999999999	10.987880000000001	9.059450000000000
N	10.755820000000000	13.031890000000001	6.916920000000000
N	10.936220000000000	8.955629999999999	6.965190000000000
N	12.826190000000000	11.098800000000001	7.084840000000000
N	8.936070000000001	10.981800000000000	7.121770000000000

Transition Metal: Co; Functional Group: BH2; Adsorbate: OH

C	10.1533200000000001	15.2684400000000000	6.6180500000000000
C	9.6833800000000000	13.8773000000000000	6.7329500000000000
C	8.3486100000000001	13.4291699999999999	6.8038400000000000
C	11.5817400000000000	6.7304300000000000	6.6888600000000000
C	12.0367400000000000	8.1365099999999999	6.7357800000000000
C	13.3472399999999999	8.6061599999999999	6.7737500000000000
C	10.1959900000000000	6.7777500000000000	6.8695800000000000
C	9.8518000000000001	8.1837700000000001	6.9367900000000000
C	11.5479900000000000	15.1869999999999999	6.7307200000000000
C	8.4987700000000000	8.5640500000000000	7.0429500000000000
C	15.1192600000000001	11.7184600000000000	7.0310400000000000
C	11.8870000000000000	13.8002500000000000	6.8477300000000000
C	13.7177799999999999	12.1831800000000000	6.9736200000000000
C	15.0358000000000000	10.3300400000000000	6.9115100000000000
C	13.6367700000000000	9.9876900000000001	6.8475800000000000
C	13.2599600000000000	13.5018700000000000	6.9295000000000000
C	6.6812500000000000	11.6677900000000000	6.9708500000000000
C	8.0741900000000000	12.0661000000000000	6.8787900000000000
C	6.6696300000000000	10.2814200000000001	7.0335300000000000
C	8.0862200000000001	9.9017599999999999	6.9844100000000000
B	9.4248300000000000	16.5607399999999999	6.2009100000000000
B	6.9640600000000000	14.2382000000000001	6.8796200000000000
B	12.2833400000000001	5.4315100000000000	6.2574000000000000
B	14.7148500000000000	7.7759100000000000	6.8248500000000000
B	9.0991800000000000	5.6410800000000000	6.8873100000000000
B	12.8248200000000001	16.1080200000000000	6.6975000000000000
B	7.4649100000000000	7.4940200000000000	7.1996400000000000
B	16.4313100000000000	12.4269000000000000	7.4284000000000000
B	15.9599400000000000	9.0566200000000001	6.9201100000000000
B	14.1005000000000000	14.8657900000000001	6.8510400000000000
B	5.7420900000000000	12.9231300000000000	6.9889500000000000
B	5.5165900000000000	9.2140100000000000	7.1176100000000000
Co	10.8646900000000000	11.0315600000000001	7.0054500000000000
H	10.6734000000000001	11.9020700000000000	9.1506799999999999
H	8.3606400000000000	16.5619100000000001	5.6457100000000000
H	9.9898900000000001	17.6105200000000001	6.3733900000000000
H	6.2220500000000000	13.7956000000000000	7.9045300000000000
H	6.7967700000000000	15.4202300000000000	6.8919900000000000
H	11.7201100000000000	4.3892400000000000	6.4859800000000000
H	13.3120200000000000	5.4038600000000000	5.6392600000000000
H	14.8557600000000000	6.5911600000000000	6.8269900000000000
H	15.5908700000000001	8.2354900000000000	5.9159400000000000
H	9.0162200000000001	4.9059300000000000	7.8428300000000000
H	8.6501400000000000	5.2342100000000000	5.8410500000000000
H	13.7034699999999999	15.6086700000000000	5.8052900000000000
H	12.9044399999999999	17.2977400000000001	6.6021500000000000
H	6.2471300000000000	7.6998400000000000	7.2653600000000000
H	7.7063400000000000	6.2839000000000000	7.3408500000000000
H	16.4571299999999999	13.4487799999999999	8.0575300000000000
H	17.4729899999999999	11.8808399999999999	7.1691400000000000
H	15.4890700000000000	8.1959400000000000	7.8406600000000000
H	17.1524600000000001	8.9812600000000001	6.9771300000000000
H	13.6381999999999999	15.7709200000000000	7.7242000000000000
H	15.2865800000000001	14.9987499999999999	6.8641200000000000
H	4.5490000000000000	12.9873600000000001	7.0682100000000000
H	6.0894600000000000	13.7642200000000000	5.9817900000000000
H	4.9635100000000000	8.8509100000000001	6.1061800000000000
H	4.9433100000000000	9.0253999999999999	8.1641999999999999
O	10.8854200000000000	10.9927899999999999	8.8588600000000000
N	10.7654800000000000	12.9928300000000000	6.8386800000000000
N	10.9417200000000000	9.0078800000000000	6.8446000000000000
N	12.8350800000000000	11.0997000000000000	6.8699200000000000
N	8.9275400000000000	10.9789600000000001	6.8721300000000000

Transition Metal: Co; Functional Group: BH2; Adsorbate: OOH

C	10.142130000000000	15.250660000000000	6.315360000000000
C	9.673320000000000	13.861590000000000	6.480210000000000
C	8.339070000000000	13.419169999999999	6.592390000000000
C	11.566150000000000	6.729620000000000	6.380710000000000
C	12.022570000000000	8.131520000000000	6.485550000000000
C	13.334130000000000	8.596869999999999	6.545510000000000
C	10.178940000000001	6.771610000000000	6.554530000000000
C	9.835200000000000	8.173450000000001	6.678020000000000
C	11.536530000000001	15.171670000000001	6.423070000000000
C	8.481930000000000	8.550750000000001	6.805040000000000
C	15.106710000000000	11.707950000000000	6.822380000000000
C	11.873690000000000	13.786980000000000	6.578930000000000
C	13.705200000000000	12.172590000000000	6.752480000000000
C	15.025140000000000	10.318519999999999	6.709540000000000
C	13.625930000000000	9.976500000000000	6.637570000000000
C	13.246400000000000	13.490550000000001	6.677140000000000
C	6.668490000000000	11.662720000000000	6.791660000000000
C	8.062419999999999	12.059340000000001	6.712760000000000
C	6.653320000000000	10.273890000000000	6.837420000000000
C	8.068140000000000	9.891159999999999	6.795110000000000
B	9.412530000000000	16.525910000000000	5.852580000000000
B	6.955940000000000	14.231520000000000	6.641760000000000
B	12.274319999999999	5.453770000000000	5.896790000000000
B	14.699960000000001	7.764270000000000	6.596790000000000
B	9.083740000000001	5.634260000000000	6.518910000000000
B	12.814240000000000	16.090280000000000	6.369520000000000
B	7.445200000000000	7.477280000000000	6.905900000000000
B	16.411320000000000	12.423999999999999	7.229460000000000
B	15.946920000000000	9.043010000000001	6.714920000000000
B	14.087890000000000	14.852140000000000	6.567490000000000
B	5.731510000000000	12.920470000000000	6.777420000000000
B	5.498090000000000	9.206310000000000	6.884050000000000
Co	10.856330000000000	11.014900000000001	6.815370000000000
H	8.341480000000001	16.506470000000000	5.310810000000000
H	9.981339999999999	17.580909999999999	5.971830000000000
H	6.207440000000000	13.815009999999999	7.673010000000000
H	6.789530000000000	15.413510000000000	6.624160000000000
H	11.710580000000000	4.400410000000000	6.065520000000000
H	13.311990000000000	5.458460000000000	5.292770000000000
H	14.840109999999999	6.579060000000000	6.589460000000000
H	15.584640000000000	8.232480000000001	5.699420000000000
H	8.992599999999999	4.863220000000000	7.444800000000000
H	8.640670000000000	5.269960000000000	5.454640000000000
H	13.698680000000000	15.564570000000000	5.497900000000000
H	12.895920000000000	17.276219999999999	6.239140000000000
H	6.227770000000000	7.687350000000000	6.977460000000000
H	7.679820000000000	6.260570000000000	6.983190000000000
H	16.422960000000000	13.452120000000001	7.848800000000000
H	17.458480000000002	11.879849999999999	6.990870000000000
H	15.467330000000000	8.174020000000001	7.622410000000000
H	17.138539999999999	8.964570000000000	6.781900000000000
H	13.619400000000001	15.781950000000000	7.410980000000000
H	15.274240000000001	14.984680000000001	6.586250000000000
H	4.538060000000000	12.988720000000001	6.851430000000000
H	6.082730000000000	13.737650000000000	5.751770000000000
H	4.943620000000000	8.878349999999999	5.861250000000000
H	4.923580000000000	8.981830000000000	7.923470000000000
H	9.453419999999999	10.630269999999999	9.610110000000001
O	11.019090000000000	11.153969999999999	8.674870000000000
O	10.303020000000000	10.171430000000001	9.417180000000000
N	10.753430000000000	12.982760000000001	6.596640000000000
N	10.927730000000000	8.999350000000000	6.622230000000000
N	12.824949999999999	11.087800000000000	6.656070000000000
N	8.913259999999999	10.968990000000000	6.721340000000000

Transition Metal: Co; Functional Group: CH3; Adsorbate: Clean

H	9.323729999999999	16.225330000000000	9.175319999999999
H	10.708360000000000	17.134950000000000	8.565790000000000
H	9.237080000000000	17.028630000000000	7.594340000000000
H	6.619140000000000	14.227000000000000	7.588880000000000
H	7.340340000000000	14.730449999999999	9.126260000000000
H	7.864250000000000	15.448779999999999	7.594170000000000
H	12.396070000000000	5.740040000000000	9.787599999999999
H	11.916869999999999	4.835020000000000	8.343740000000000
H	13.404489999999999	5.783590000000000	8.331910000000000
H	14.711560000000000	8.842309999999999	10.161550000000000
H	13.445160000000000	7.629410000000000	10.331000000000000
H	14.758139999999999	7.375070000000000	9.169499999999999
H	9.611179999999999	5.374380000000000	6.087050000000000
H	10.068390000000000	4.768270000000000	7.686290000000000
H	8.582240000000000	5.699770000000000	7.491630000000000
H	12.244540000000000	17.229579999999999	7.293190000000000
H	13.644250000000000	16.155909999999999	7.126120000000000
H	12.684200000000000	16.601500000000000	5.704780000000000
H	8.565370000000000	7.142530000000000	5.176270000000000
H	7.232310000000000	7.095420000000000	6.342030000000000
H	7.295780000000000	8.363230000000000	5.106150000000000
H	16.376239999999999	13.322369999999999	6.765940000000000
H	17.257560000000000	11.795690000000000	6.841040000000000
H	16.414899999999999	12.254619999999999	5.353340000000000
H	16.555910000000000	9.730570000000000	9.252879999999999
H	16.233870000000000	8.577439999999999	7.946880000000000
H	17.226790000000000	10.003130000000000	7.637900000000000
H	14.852060000000000	14.683100000000000	5.829270000000000
H	14.602209999999999	13.367430000000000	4.670090000000000
H	13.432490000000000	14.682130000000000	4.768330000000000
H	4.873610000000000	11.448210000000000	8.663679999999999
H	5.816350000000000	12.829400000000000	9.226860000000000
H	5.031310000000000	12.876180000000000	7.635590000000000
H	5.789010000000000	8.431630000000000	7.506980000000000
H	4.749410000000000	9.865970000000000	7.473150000000000
H	5.415760000000000	9.229749999999999	5.969780000000000
C	10.473100000000000	15.209420000000000	7.632230000000000
C	9.959410000000000	13.838110000000000	7.676570000000000
C	8.617330000000000	13.433500000000000	7.888540000000000
C	11.585680000000000	6.961170000000000	8.166589999999999
C	11.972300000000000	8.370889999999999	8.204920000000000
C	13.234500000000000	8.884380000000000	8.588010000000000
C	10.401130000000000	6.888940000000000	7.449650000000000
C	10.005760000000000	8.262980000000000	7.149270000000000
C	11.712389999999999	15.156240000000000	7.015450000000000
C	8.745580000000000	8.689399999999999	6.670980000000000
C	15.114920000000000	11.562030000000000	6.965610000000000
C	12.021310000000000	13.747170000000000	6.812360000000000
C	13.720990000000000	11.976369999999999	6.820360000000000
C	15.113659999999999	10.429980000000000	7.766390000000000
C	13.714790000000000	10.088170000000000	8.015580000000000
C	13.258540000000000	13.227050000000000	6.353370000000000
C	6.813760000000000	11.592150000000000	7.740570000000000
C	8.192200000000000	12.089130000000000	7.739050000000000
C	6.844230000000000	10.314109999999999	7.207530000000000
C	8.247660000000000	9.971209999999999	7.015620000000000
C	9.897380000000000	16.453890000000000	8.267590000000000
C	7.559180000000000	14.512720000000000	8.066400000000000
C	12.362539999999999	5.778210000000000	8.686299999999999
C	14.087270000000000	8.136530000000000	9.599930000000000
C	9.629280000000000	5.626440000000000	7.160420000000000
C	12.617640000000000	16.336700000000000	6.773280000000000
C	7.910620000000000	7.769570000000000	5.794540000000000
C	16.344909999999999	12.267160000000000	6.453350000000000
C	16.336970000000000	9.648770000000000	8.175060000000000
C	14.086100000000000	14.037910000000000	5.369300000000000

C	5.580100000000000	12.226640000000000	8.340170000000001
C	5.647800000000000	9.414529999999999	7.031410000000000
Co	10.967190000000000	11.053540000000000	7.400430000000000
N	10.973000000000001	12.969849999999999	7.273940000000000
N	10.984349999999999	9.133319999999999	7.601250000000000
N	12.898080000000000	11.043640000000000	7.434670000000000
N	9.042970000000000	11.043310000000000	7.385790000000000

Transition Metal: Co; Functional Group: CH3; Adsorbate: O

H	9.336349999999999	16.153890000000001	9.214020000000000
H	10.736200000000000	17.075980000000001	8.659509999999999
H	9.277559999999999	17.017260000000000	7.663890000000000
H	6.639590000000000	14.208130000000001	7.563380000000000
H	7.364140000000000	14.713699999999999	9.099140000000000
H	7.887130000000000	15.429510000000001	7.565040000000000
H	12.332810000000000	5.789690000000000	9.834110000000001
H	11.882870000000000	4.852160000000000	8.401520000000000
H	13.371460000000001	5.798660000000000	8.398320000000000
H	14.655040000000000	8.898429999999999	10.148400000000001
H	13.387549999999999	7.687410000000000	10.316599999999999
H	14.721790000000000	7.413540000000000	9.183949999999999
H	9.563110000000000	5.350150000000000	6.124820000000000
H	10.029059999999999	4.768080000000000	7.730870000000000
H	8.548299999999999	5.709080000000000	7.531620000000000
H	12.270619999999999	17.218570000000000	7.358840000000000
H	13.669750000000001	16.147240000000000	7.165860000000000
H	12.712160000000001	16.629890000000000	5.755000000000000
H	8.530530000000001	7.122410000000000	5.132220000000000
H	7.214420000000000	7.076510000000000	6.319660000000000
H	7.257970000000000	8.341139999999999	5.077130000000000
H	16.378779999999999	13.357080000000000	6.808940000000000
H	17.272279999999999	11.836300000000000	6.886030000000000
H	16.454590000000000	12.304180000000001	5.386640000000000
H	16.515450000000001	9.787350000000000	9.297400000000000
H	16.229970000000002	8.610989999999999	8.002940000000001
H	17.222980000000000	10.036170000000000	7.694130000000000
H	14.872010000000000	14.703170000000000	5.808720000000000
H	14.624919999999999	13.405559999999999	4.626420000000000
H	13.456030000000000	14.720359999999999	4.740370000000000
H	4.932790000000000	11.429530000000000	8.757260000000000
H	5.890560000000000	12.822430000000001	9.264889999999999
H	5.042340000000000	12.845530000000000	7.705840000000000
H	5.798840000000000	8.413309999999999	7.540230000000000
H	4.758020000000000	9.848360000000000	7.537650000000000
H	5.385260000000000	9.215199999999999	6.015210000000000
C	10.498290000000001	15.190460000000000	7.647320000000000
C	9.979690000000000	13.820779999999999	7.645350000000000
C	8.637680000000000	13.414300000000001	7.857240000000000
C	11.557750000000000	6.972200000000000	8.166689999999999
C	11.951810000000000	8.381970000000001	8.157410000000000
C	13.208460000000001	8.907880000000000	8.546090000000000
C	10.374370000000001	6.882060000000000	7.447250000000000
C	9.989720000000000	8.246510000000001	7.097810000000000
C	11.736390000000000	15.154940000000000	7.023580000000000
C	8.728840000000000	8.671530000000001	6.616800000000000
C	15.128170000000001	11.586600000000001	6.959840000000000
C	12.037340000000000	13.753170000000001	6.767230000000000
C	13.738099999999999	11.989599999999999	6.766150000000000
C	15.107279999999999	10.454750000000001	7.763180000000000
C	13.701520000000000	10.103780000000000	7.965220000000000
C	13.276630000000001	13.241730000000000	6.299020000000000
C	6.832500000000000	11.573029999999999	7.753250000000000
C	8.209490000000001	12.071050000000000	7.706250000000000
C	6.844120000000000	10.296070000000000	7.213130000000000
C	8.239060000000000	9.955819999999999	6.969520000000000
C	9.924390000000001	16.413360000000001	8.324410000000000
C	7.580920000000000	14.494199999999999	8.039429999999999
C	12.322929999999999	5.802370000000000	8.731629999999999
C	14.042350000000001	8.181680000000000	9.588400000000000
C	9.591939999999999	5.619740000000000	7.193170000000000
C	12.644130000000001	16.339390000000002	6.816380000000000
C	7.882670000000000	7.749280000000000	5.758000000000000
C	16.364220000000000	12.304910000000000	6.484720000000000
C	16.322780000000002	9.685900000000000	8.216320000000000
C	14.107590000000000	14.066860000000000	5.333630000000000

C	5.621430000000000	12.207530000000000	8.396459999999999
C	5.643830000000000	9.397100000000000	7.070920000000000
Co	10.971500000000001	11.022670000000000	7.010240000000000
O	10.996869999999999	10.865580000000000	5.278070000000000
N	10.988799999999999	12.974320000000001	7.206900000000000
N	10.970520000000000	9.116110000000001	7.522050000000000
N	12.910670000000000	11.053890000000001	7.352360000000000
N	9.036910000000001	11.024710000000001	7.320870000000000

Transition Metal: Co; Functional Group: CH3; Adsorbate: OH

H	10.3957200000000001	11.5663500000000000	5.0695800000000000
H	9.3259100000000000	16.2075400000000002	9.1898000000000000
H	10.7278000000000000	17.1149700000000000	8.6169400000000000
H	9.2717500000000001	17.0356099999999998	7.6198100000000000
H	6.6308300000000000	14.2231400000000001	7.5711300000000000
H	7.3474200000000000	14.7440400000000000	9.1051400000000000
H	7.8766200000000000	15.4475200000000001	7.5673900000000000
H	12.3572900000000001	5.7716700000000000	9.8169400000000001
H	11.8834700000000001	4.8521800000000000	8.3809700000000000
H	13.3810199999999999	5.7848900000000000	8.3710700000000000
H	14.7037600000000001	8.8521000000000000	10.1578900000000000
H	13.4341700000000000	7.6418600000000000	10.3239699999999999
H	14.7477500000000000	7.3862000000000000	9.1637400000000001
H	9.5923800000000000	5.3935800000000000	6.0860600000000000
H	10.0434900000000000	4.7866100000000000	7.6872900000000000
H	8.5677100000000000	5.7347000000000000	7.4904400000000000
H	12.2761999999999999	17.2210500000000002	7.3355400000000000
H	13.6684800000000001	16.1393899999999999	7.1544000000000000
H	12.7128800000000000	16.6111900000000001	5.7385700000000000
H	8.6000599999999999	7.1913700000000000	5.1063800000000000
H	7.2614500000000000	7.1188400000000000	6.2673000000000000
H	7.3246600000000000	8.4091500000000000	5.0530200000000000
H	16.3740600000000000	13.3468100000000000	6.7948800000000000
H	17.2661799999999999	11.8259899999999999	6.8707200000000000
H	16.4287199999999998	12.2831899999999999	5.3791100000000000
H	16.5472100000000000	9.7564800000000000	9.2853300000000000
H	16.2415799999999999	8.6003300000000000	7.9777800000000000
H	17.2315000000000000	10.0293100000000001	7.6761700000000000
H	14.8533200000000000	14.6710600000000001	5.7911000000000000
H	14.5818200000000000	13.3546000000000000	4.6353200000000000
H	13.4200900000000000	14.6774299999999999	4.7467900000000000
H	4.9133900000000000	11.4350900000000001	8.7210800000000001
H	5.8519200000000000	12.8344799999999999	9.2465300000000000
H	5.0339100000000000	12.8507300000000000	7.6707600000000000
H	5.8301700000000000	8.4203800000000000	7.5215700000000000
H	4.7754500000000000	9.8447200000000001	7.5125300000000000
H	5.4240400000000000	9.2220900000000000	5.9945900000000000
C	10.4907000000000000	15.2063799999999999	7.6481700000000000
C	9.9721800000000000	13.8388899999999999	7.6807000000000000
C	8.6293300000000000	13.4360000000000000	7.8842800000000000
C	11.5751399999999999	6.9773600000000000	8.1698100000000000
C	11.9701000000000000	8.3861399999999999	8.1943600000000000
C	13.2310099999999999	8.8976200000000000	8.5804899999999999
C	10.3979900000000000	6.9037500000000000	7.4407400000000000
C	10.0159900000000000	8.2765200000000000	7.1228800000000000
C	11.7299100000000000	15.1555800000000000	7.0282800000000000
C	8.7659100000000000	8.7092899999999999	6.6269700000000000
C	15.1235000000000000	11.5785000000000000	6.9792200000000000
C	12.0309399999999999	13.7492199999999999	6.8071200000000000
C	13.7303900000000000	11.9856099999999999	6.8188700000000000
C	15.1166800000000001	10.4481500000000000	7.7825800000000000
C	13.7149500000000000	10.1027000000000000	8.0152300000000001
C	13.2614500000000000	13.2250599999999999	6.3331300000000000
C	6.8320900000000000	11.5888899999999999	7.7553400000000000
C	8.2066400000000000	12.0914199999999999	7.7426100000000000
C	6.8616200000000000	10.3133400000000000	7.2136700000000000
C	8.2624700000000000	9.9805400000000000	7.0003900000000000
C	9.9161000000000000	16.4453500000000001	8.2952999999999999
C	7.5694300000000000	14.5159100000000000	8.0482600000000001
C	12.3357100000000001	5.7952800000000000	8.7150000000000000
C	14.0787499999999999	8.1483800000000000	9.5950399999999999
C	9.6137999999999999	5.6478000000000000	7.1585600000000000
C	12.6435000000000000	16.3327999999999999	6.8033600000000000
C	7.9386100000000000	7.8038900000000000	5.7320700000000000
C	16.3527200000000001	12.2922600000000001	6.4785800000000000
C	16.3383100000000000	9.6721800000000001	8.2058300000000001

C	14.078920000000000	14.030430000000001	5.339070000000000
C	5.604210000000000	12.217269999999999	8.373139999999999
C	5.670650000000000	9.404080000000000	7.053300000000000
Co	10.975370000000000	11.053540000000000	7.246220000000000
O	11.018129999999999	10.885930000000000	5.393940000000000
N	10.988429999999999	12.971030000000001	7.277990000000000
N	10.985740000000000	9.146080000000000	7.581440000000000
N	12.904650000000000	11.061550000000000	7.433180000000000
N	9.058059999999999	11.045190000000000	7.387290000000000

Transition Metal: Co; Functional Group: CH3; Adsorbate: OOH

H	9.298780000000001	16.164510000000000	9.375109999999999
H	10.710889999999999	17.077410000000000	8.835770000000000
H	9.262480000000000	17.028949999999998	7.824660000000000
H	6.617440000000000	14.211050000000000	7.678590000000000
H	7.312870000000000	14.749950000000000	9.216780000000000
H	7.867720000000000	15.432020000000000	7.678060000000000
H	12.318759999999999	5.784040000000000	10.018680000000000
H	11.864179999999999	4.850570000000000	8.585880000000000
H	13.356780000000001	5.791680000000000	8.582900000000000
H	14.661339999999999	8.874730000000000	10.326700000000001
H	13.397800000000000	7.659250000000000	10.494160000000001
H	14.720490000000000	7.401590000000000	9.344379999999999
H	9.536420000000000	5.367230000000000	6.304230000000000
H	10.031010000000000	4.767910000000000	7.894460000000000
H	8.543410000000000	5.702770000000000	7.732670000000000
H	12.264480000000001	17.207719999999998	7.539040000000000
H	13.652160000000000	16.120560000000001	7.351630000000000
H	12.705539999999999	16.613060000000001	5.936910000000000
H	8.528269999999999	7.143100000000000	5.315480000000000
H	7.222230000000000	7.068970000000000	6.511230000000000
H	7.236370000000000	8.344860000000001	5.282910000000000
H	16.342680000000001	13.354229999999999	6.986590000000000
H	17.240720000000000	11.836090000000000	7.045710000000000
H	16.408570000000001	12.310930000000001	5.556510000000000
H	16.500969999999999	9.797100000000000	9.481579999999999
H	16.230280000000000	8.618420000000000	8.186529999999999
H	17.207820000000002	10.055690000000000	7.880330000000000
H	14.827620000000000	14.676399999999999	5.948280000000000
H	14.555429999999999	13.362760000000000	4.789020000000000
H	13.390390000000000	14.682060000000000	4.907780000000000
H	4.904250000000000	11.443390000000001	8.933100000000000
H	5.856080000000000	12.848520000000001	9.417650000000000
H	5.006000000000000	12.843660000000000	7.859530000000000
H	5.794340000000000	8.410720000000000	7.747210000000000
H	4.741880000000000	9.836639999999999	7.741530000000000
H	5.359110000000000	9.194760000000000	6.219120000000000
H	9.365000000000000	11.265960000000000	4.750240000000000
C	10.471550000000001	15.192729999999999	7.821720000000000
C	9.953780000000000	13.822380000000001	7.838090000000000
C	8.608870000000000	13.422739999999999	8.028370000000001
C	11.545210000000001	6.972080000000000	8.356500000000000
C	11.938390000000000	8.381090000000000	8.359410000000000
C	13.199479999999999	8.899270000000000	8.738810000000001
C	10.363149999999999	6.886620000000000	7.635870000000000
C	9.976990000000001	8.254030000000000	7.302730000000000
C	11.710640000000000	15.147990000000000	7.205000000000000
C	8.718660000000000	8.679110000000000	6.817140000000000
C	15.098190000000001	11.579689999999999	7.139840000000000
C	12.011559999999999	13.741989999999999	6.972280000000000
C	13.705230000000000	11.978400000000001	6.961820000000000
C	15.087800000000000	10.452680000000001	7.948290000000000
C	13.685269999999999	10.098640000000000	8.163830000000001
C	13.239360000000000	13.224750000000000	6.488180000000000
C	6.804070000000000	11.580640000000001	7.926320000000000
C	8.180400000000001	12.077640000000001	7.894940000000000
C	6.822590000000000	10.298730000000001	7.398680000000000
C	8.220940000000001	9.958060000000000	7.174880000000000
C	9.898170000000000	16.420079999999999	8.491560000000000
C	7.549840000000000	14.507529999999999	8.166510000000001
C	12.308330000000000	5.798570000000000	8.916410000000001
C	14.044190000000000	8.163040000000001	9.765370000000001
C	9.581659999999999	5.624360000000000	7.375030000000000
C	12.629810000000001	16.323889999999999	6.998210000000000
C	7.877240000000000	7.756230000000000	5.951920000000000
C	16.327510000000000	12.304020000000000	6.655330000000000
C	16.310549999999999	9.694570000000001	8.400180000000001

C	14.053310000000000	14.035660000000000	5.496270000000000
C	5.589020000000000	12.218920000000001	8.558990000000000
C	5.627420000000000	9.389130000000000	7.270490000000000
Co	10.945650000000001	11.040699999999999	7.375920000000000
O	11.024229999999999	10.764230000000000	5.532620000000000
O	10.253030000000001	11.687790000000000	4.741590000000000
N	10.970829999999999	12.960100000000001	7.434940000000000
N	10.951480000000000	9.130549999999999	7.738880000000000
N	12.877420000000001	11.049099999999999	7.563310000000000
N	9.022980000000000	11.028620000000000	7.537320000000000

Transition Metal: Co; Functional Group: F; Adsorbate: Clean

Co	0.000000000000000	-0.000109965181886	0.000524276009998
C	0.681577492909118	4.237384941309096	-0.008097484387807
C	1.101851218368110	2.854153436237326	-0.006076499916618
C	2.421261431806436	2.429549328694154	-0.000590987177066
C	-0.681586433504197	-4.237450143081489	-0.007524253658669
C	-1.101901071525166	-2.854231662524395	-0.003321607470284
C	-2.421383146175597	-2.429641010885195	-0.000481747093568
C	0.681586433504196	-4.237450143081489	-0.007524253658669
C	1.101901071525170	-2.854231662524395	-0.003321607470284
C	-0.681577492909117	4.237384941309096	-0.008097484387807
C	2.421383146175602	-2.429641010885195	-0.000481747093568
C	-4.221651425349048	0.686556972408146	0.004957250189542
C	-1.101851218368108	2.854153436237326	-0.006076499916618
C	-2.849915877970663	1.106147628306420	0.005285258377556
C	-4.221809099557241	-0.686318938321524	0.004701486489498
C	-2.850082888427629	-1.106208168856689	0.005142231890914
C	-2.421261431806442	2.429549328694154	-0.000590987177066
C	4.221651425349050	0.686556972408146	0.004957250189542
C	2.849915877970664	1.106147628306420	0.005285258377556
C	4.221809099557240	-0.686318938321524	0.004701486489498
C	2.850082888427628	-1.106208168856689	0.005142231890914
N	0.000000000000000	1.999850565257888	-0.005741888053396
N	0.000000000000000	-1.999956858851867	-0.001489794762074
N	-1.997071124840808	-0.000078106410420	0.006148317378864
N	1.997071124840806	-0.000078106410420	0.006148317378864
F	5.309071429480628	-1.475585369756175	0.001915690743732
F	-5.308636107776895	1.476169006362696	0.002208859962122
F	-5.309071429480628	-1.475585369756175	0.001915690743732
F	-1.483491383870668	5.317208223615451	-0.004216747717056
F	1.483491383870670	5.317208223615451	-0.004216747717056
F	5.308636107776898	1.476169006362696	0.002208859962122
F	-1.483448535292450	-5.317284600853798	-0.006692513586064
F	1.483448535292450	-5.317284600853798	-0.006692513586064
F	-3.386910431444146	3.390132272796416	0.000027300391166
F	3.386910431444146	3.390132272796416	0.000027300391166
F	-3.387096151904935	-3.390185679651982	-0.003185851013768
F	3.387096151904934	-3.390185679651982	-0.003185851013768

Transition Metal: Co; Functional Group: F; Adsorbate: O

Co	0.000000000000000	-0.000501774070820	0.439511860568916
C	0.685786067003130	4.270921665631372	-0.001872960496446
C	1.106554363507490	2.888914202317346	-0.015530422678434
C	2.430389154863860	2.429292355198998	-0.014202900631662
C	-0.685721542112944	-4.272779226808108	-0.002125917602866
C	-1.106361568695370	-2.890633876756525	-0.015786202604396
C	-2.430191570780124	-2.431051757168692	-0.014373209612370
C	0.685721542112940	-4.272779226808108	-0.002125917602866
C	1.106361568695372	-2.890633876756525	-0.015786202604396
C	-0.685786067003139	4.270921665631372	-0.001872960496446
C	2.430191570780128	-2.431051757168692	-0.014373209612370
C	-4.272287292528560	0.684781780389900	-0.004220938753651
C	-1.106554363507495	2.888914202317346	-0.015530422678434
C	-2.890234599144847	1.105516672205156	-0.016062451359407
C	-4.272494812269816	-0.686714737307945	-0.004268827825939
C	-2.890200196121128	-1.107291673554293	-0.016128076067435
C	-2.430389154863857	2.429292355198998	-0.014202900631662
C	4.272287292528568	0.684781780389900	-0.004220938753651
C	2.890234599144840	1.105516672205156	-0.016062451359407
C	4.272494812269819	-0.686714737307945	-0.004268827825939
C	2.890200196121130	-1.107291673554293	-0.016128076067435
N	0.000000000000000	2.054315660353932	-0.035181509765636
N	0.000000000000000	-2.055807554625375	-0.035406737186886
N	-2.055501515165723	-0.000819649780784	-0.035124071861599
N	2.055501515165726	-0.000819649780784	-0.035124071861599
F	5.359965417520630	-1.478188599600760	-0.001706286500864
F	-5.359549288533428	1.476338063043396	-0.001667811284612
F	-5.359965417520629	-1.478188599600760	-0.001706286500864
F	-1.477117381243946	5.358442079822085	0.000353877631084
F	1.477117381243948	5.358442079822085	0.000353877631084
F	5.359549288533438	1.476338063043396	-0.001667811284612
F	-1.477123054101771	-5.360184453760555	0.000250306331316
F	1.477123054101774	-5.360184453760555	0.000250306331316
F	-3.391510235928482	3.390614338167460	0.000028899086172
F	3.391510235928484	3.390614338167460	0.000028899086172
F	-3.391516413291786	-3.392279270527752	-0.000142489729750
F	3.391516413291794	-3.392279270527752	-0.000142489729750
O	0.000000000000000	-0.001382154678488	2.085105354304592

Transition Metal: Co; Functional Group: F; Adsorbate: OH

Co	0.000000000000000	0.003532914510670	0.147322936370412
C	0.683496943207020	4.233296241545370	0.005722041839448
C	1.104432445086512	2.854742353368304	0.010979015958224
C	2.426350902636066	2.425092427599272	0.011631786577996
C	-0.683033484712350	-4.230547392191603	0.002827178464984
C	-1.101575446280666	-2.849664952397223	-0.002052912624684
C	-2.422638936063585	-2.418936239597819	0.014879423601040
C	0.683033484712356	-4.230547392191603	0.002827178464984
C	1.101575446280674	-2.849664952397223	-0.002052912624684
C	-0.683496943207022	4.233296241545370	0.005722041839448
C	2.422638936063580	-2.418936239597819	0.014879423601040
C	-4.238228563548564	0.685206240711328	0.007669690277344
C	-1.104432445086513	2.854742353368304	0.010979015958224
C	-2.857896175575117	1.104913233184716	-0.004076026988672
C	-4.236556947378761	-0.680914168903225	0.010848746189114
C	-2.855047006562529	-1.098400184155821	0.000983654727088
C	-2.426350902636063	2.425092427599272	0.011631786577996
C	4.238228563548560	0.685206240711328	0.007669690277344
C	2.857896175575116	1.104913233184716	-0.004076026988672
C	4.236556947378761	-0.680914168903225	0.010848746189114
C	2.855047006562530	-1.098400184155821	0.000983654727088
N	0.000000000000000	2.003000491099544	0.000691792075134
N	0.000000000000000	-2.001610240910978	-0.027107433154500
N	-2.007500354658820	0.003779307946980	-0.031448993306647
N	2.007500354658820	0.003779307946980	-0.031448993306647
F	5.317055740981655	-1.480759802142579	0.005503246565844
F	-5.320095950980189	1.483651507407416	0.001708271899696
F	-5.317055740981655	-1.480759802142579	0.005503246565844
F	-1.481159799172751	5.315391903592076	-0.010960217055281
F	1.481159799172750	5.315391903592076	-0.010960217055281
F	5.320095950980192	1.483651507407416	0.001708271899696
F	-1.482057640689924	-5.311632937623244	-0.006263350296287
F	1.482057640689926	-5.311632937623244	-0.006263350296287
F	-3.386146145474143	3.388352291776720	0.028525396161692
F	3.386146145474148	3.388352291776720	0.028525396161692
F	-3.383334666796671	-3.380434985041006	0.042989483832698
F	3.383334666796668	-3.380434985041006	0.042989483832698
H	0.000000000000000	0.856202397678692	2.316382807498008
O	0.000000000000000	-0.070275252537005	2.003407025563156

Transition Metal: Co; Functional Group: F; Adsorbate: OOH

Co	-0.000879610980182	0.001232206009978	0.165048281344990
C	0.683970501562494	4.240936812524218	0.003896090491342
C	1.101892333758310	2.859570510232148	0.000367227267644
C	2.423213835902650	2.427216089971804	0.009053927762402
C	-0.682185269750821	-4.230915646262641	0.012276719111752
C	-1.101053772646573	-2.849799034533692	0.010713278719618
C	-2.421714611839995	-2.417535000610581	0.020232019728754
C	0.683696527871612	-4.230971867086890	0.011791618620920
C	1.103127881459234	-2.849917425524641	0.009362016674844
C	-0.682156285217292	4.242643539131910	0.003152739823444
C	2.424361906432544	-2.418930780427260	0.014368224451090
C	-4.237297960859864	0.689384569634310	0.000954716057190
C	-1.103146713183023	2.862362540949262	-0.001260647421222
C	-2.857725958797054	1.110831617339904	-0.001209980060376
C	-4.235847887606283	-0.677616098219779	0.003727233529228
C	-2.855485967704201	-1.096167010552424	0.004596085732396
C	-2.425018700457432	2.432204038223902	0.007285547439788
C	4.237128830699445	0.687456018690052	0.000426043204340
C	2.856048741737948	1.106291548549648	-0.006767452354673
C	4.237176016750260	-0.678743506395271	0.001909706010888
C	2.856299991374552	-1.097678296323409	-0.003704586989470
N	-0.001335762776630	2.012283075246322	-0.018911491180136
N	0.000990751475828	-2.002019733163060	-0.007000309814050
N	-2.008158915543525	0.007349089516436	-0.011325870130435
N	2.008747893808716	0.003927704784868	-0.029682055519949
F	5.319047129950626	-1.477219625777067	-0.002820350261900
F	-5.320905248666817	1.486086356230182	-0.007800795736494
F	-5.317907047790449	-1.476200432265632	-0.004281645298718
F	-1.479375237798088	5.325755789570547	-0.005083412882332
F	1.482948949583072	5.322183770733796	-0.003334408759934
F	5.318846716085704	1.486029162501444	-0.003170226813790
F	-1.481468899363605	-5.312203570572889	-0.000024086290559
F	1.482462896208186	-5.312389674389467	-0.001160501171611
F	-3.387504664822242	3.394826759953508	0.023745232760870
F	3.384981114202148	3.389429987508996	0.030496190667216
F	-3.384227014731252	-3.378808427564515	0.036260590392042
F	3.386015120865316	-3.380702965689061	0.034149060741832
H	-1.491048163501873	-0.072384886847281	2.963905347785876
O	0.156272848625532	0.079366818490836	2.033226310182382
O	-0.779590419516897	-0.719268535088531	2.752706226295098

Transition Metal: Co; Functional Group: H; Adsorbate: Clean

Co	0.000000000000000	-0.000071483714636	0.006950531754042
C	0.683728354050244	4.224039241054466	-0.009946648290711
C	1.101363985106156	2.839683703581576	-0.004064535392132
C	2.429366084304466	2.429231467053032	0.000480553581304
C	-0.683789141246514	-4.224009081931449	-0.007592673972390
C	-1.101564832937012	-2.839732908827798	0.000139862318244
C	-2.429668245739862	-2.429316918842840	0.002360916487830
C	0.683789141246520	-4.224009081931449	-0.007592673972390
C	1.101564832937008	-2.839732908827798	0.000139862318244
C	-0.683728354050256	4.224039241054466	-0.009946648290711
C	2.429668245739868	-2.429316918842840	0.002360916487830
C	-4.224709246265991	0.683846675166218	0.004171405521068
C	-1.101363985106158	2.839683703581576	-0.004064535392132
C	-2.840271205042910	1.101327731150890	0.006100413325138
C	-4.224886709068819	-0.683685959014312	0.004205564785532
C	-2.840614482460147	-1.101528902747670	0.006594589598254
C	-2.429366084304473	2.429231467053032	0.000480553581304
C	4.224709246265986	0.683846675166218	0.004171405521068
C	2.840271205042912	1.101327731150890	0.006100413325138
C	4.224886709068822	-0.683685959014312	0.004205564785532
C	2.840614482460146	-1.101528902747670	0.006594589598254
N	0.000000000000000	1.991162193796222	-0.001108829961780
N	0.000000000000000	-1.991368013637242	0.004243985478442
N	-1.991896334362600	-0.000199295856364	0.008342066781928
N	1.991896334362602	-0.000199295856364	0.008342066781928
H	5.074432743706097	-1.363982761823685	0.000385870052382
H	-5.073682542169553	1.365046788469428	0.000174666177850
H	-5.074432743706108	-1.363982761823685	0.000385870052382
H	-1.364741832675243	5.073021110207469	-0.012660953055295
H	1.364741832675250	5.073021110207469	-0.012660953055295
H	5.073682542169560	1.365046788469428	0.000174666177850
H	-1.364619377884114	-5.073161512338780	-0.013254200449321
H	1.364619377884116	-5.073161512338780	-0.013254200449321
H	-3.201086787553368	3.201051335291118	-0.001793730739626
H	3.201086787553374	3.201051335291118	-0.001793730739626
H	-3.201062627185802	-3.201282058813355	-0.001841010365678
H	3.201062627185806	-3.201282058813355	-0.001841010365678

Transition Metal: Co; Functional Group: H; Adsorbate: O

Co	0.000000000000000	-0.000672129047754	0.308430638567544
C	0.684221625024364	4.226081385130924	-0.022518582805461
C	1.102913741530416	2.841734970254220	0.004898731998616
C	2.432105379565518	2.429723433349330	0.013900997576972
C	-0.684205315548503	-4.228024727464788	-0.022436259470197
C	-1.102973916561908	-2.843727439303663	0.006359386744288
C	-2.432286210662873	-2.432034642225087	0.013984419710940
C	0.684205315548502	-4.228024727464788	-0.022436259470197
C	1.102973916561910	-2.843727439303663	0.006359386744288
C	-0.684221625024367	4.226081385130924	-0.022518582805461
C	2.432286210662874	-2.432034642225087	0.013984419710940
C	-4.231761240023847	0.683292680971560	-0.011791634164297
C	-1.102913741530422	2.841734970254220	0.004898731998616
C	-2.846893200953762	1.101319032990916	0.010610558161976
C	-4.231971167268838	-0.685248560719490	-0.011885327724904
C	-2.847170193697334	-1.103666065614178	0.010562200547330
C	-2.432105379565520	2.429723433349330	0.013900997576972
C	4.231761240023854	0.683292680971560	-0.011791634164297
C	2.846893200953768	1.101319032990916	0.010610558161976
C	4.231971167268838	-0.685248560719490	-0.011885327724904
C	2.847170193697334	-1.103666065614178	0.010562200547330
N	0.000000000000000	2.005422477866288	0.010559138239278
N	0.000000000000000	-2.007327898703203	0.013626352796786
N	-2.011173976134046	-0.001235669920670	0.014984350583750
N	2.011173976134034	-0.001235669920670	0.014984350583750
H	5.081165093340609	-1.365790262102632	-0.028400835480145
H	-5.080544277767441	1.364339640505624	-0.028565125132161
H	-5.081165093340612	-1.365790262102632	-0.028400835480145
H	-1.365389083767951	5.074579407537916	-0.040968143936077
H	1.365389083767952	5.074579407537916	-0.040968143936077
H	5.080544277767432	1.364339640505624	-0.028565125132161
H	-1.365202280585521	-5.076652342937731	-0.041795546540378
H	1.365202280585536	-5.076652342937731	-0.041795546540378
H	-3.202655052352625	3.202190659378256	0.012802848631704
H	3.202655052352628	3.202190659378256	0.012802848631704
H	-3.202543042471476	-3.204779853314975	0.011259644010402
H	3.202543042471478	-3.204779853314975	0.011259644010402
O	0.000000000000000	0.004754256853828	2.054250504971068

Transition Metal: Co; Functional Group: H; Adsorbate: OH

Co	0.000000000000000	0.002812900979870	0.148003883738048
C	0.684159124878012	4.222150299949842	-0.001380731506526
C	1.102254698354390	2.839488800637204	0.014229503855644
C	2.430089565603152	2.428174498334828	0.017462445922956
C	-0.683491785011672	-4.221830927384518	-0.003503093099493
C	-1.099498805780939	-2.836393285839925	0.006626354192350
C	-2.426524092065460	-2.425347674528968	0.019228732802010
C	0.683491785011668	-4.221830927384518	-0.003503093099493
C	1.099498805780936	-2.836393285839925	0.006626354192350
C	-0.684159124878004	4.222150299949842	-0.001380731506526
C	2.426524092065460	-2.425347674528968	0.019228732802010
C	-4.225954471692134	0.683503985835450	0.001155647992912
C	-1.102254698354386	2.839488800637204	0.014229503855644
C	-2.841002400776983	1.101166301415486	0.003663391830892
C	-4.223626687974898	-0.683565284564033	0.004035867254290
C	-2.837779034511740	-1.098134903684798	0.007409280953744
C	-2.430089565603140	2.428174498334828	0.017462445922956
C	4.225954471692140	0.683503985835450	0.001155647992912
C	2.841002400776992	1.101166301415486	0.003663391830892
C	4.223626687974892	-0.683565284564033	0.004035867254290
C	2.837779034511748	-1.098134903684798	0.007409280953744
N	0.000000000000000	1.990081741256506	0.012158658966112
N	0.000000000000000	-1.989897192981292	-0.004693348813334
N	-1.992518516163827	0.002106641971196	-0.012015385046324
N	1.992518516163834	0.002106641971196	-0.012015385046324
H	5.070566097783850	-1.367102509390932	0.000526161849244
H	-5.075056429018456	1.364306542549306	-0.004881928275836
H	-5.070566097783855	-1.367102509390932	0.000526161849244
H	-1.365678315495728	5.070597500611126	-0.017073290370085
H	1.365678315495724	5.070597500611126	-0.017073290370085
H	5.075056429018452	1.364306542549306	-0.004881928275836
H	-1.365583650086762	-5.069868067158643	-0.013876431763023
H	1.365583650086770	-5.069868067158643	-0.013876431763023
H	-3.201261926199066	3.200654348954232	0.027527635921806
H	3.201261926199066	3.200654348954232	0.027527635921806
H	-3.198421851566650	-3.196954303611545	0.035002325201606
H	3.198421851566656	-3.196954303611545	0.035002325201606
H	0.000000000000000	0.892350398405750	2.289124928013028
O	0.000000000000000	-0.044131775851241	2.006762902663170

Transition Metal: Co; Functional Group: H; Adsorbate: OOH

Co	-0.000373992436430	0.025517527893046	0.182552681251728
C	0.694891762790590	4.251205730206943	0.034151548488928
C	1.105480054758720	2.864471052571320	0.024553834902264
C	2.431553824802736	2.447620990409836	-0.000936665304132
C	-0.697795046312240	-4.192485967144830	0.133538234693834
C	-1.110080498133975	-2.806436574624371	0.096977473564410
C	-2.435964480137201	-2.390796873441353	0.078091601582012
C	0.669147264519270	-4.197158206209954	0.121291688597772
C	1.089977418508454	-2.813546725048603	0.076800346918424
C	-0.672410916660510	4.256936951900642	0.030020060120440
C	2.418171037831152	-2.406768288566983	0.032425122838194
C	-4.223612860135050	0.725495401419106	-0.063664882811548
C	-1.094542364396066	2.873390056789850	0.021499333173898
C	-2.839523616707687	1.140158645734782	-0.015689145988690
C	-4.226675678471041	-0.642768551054679	-0.041299366829087
C	-2.844897259037033	-1.062643966540108	0.019235022615752
C	-2.423930756065399	2.467130004548762	0.004679740695906
C	4.221028133688890	0.698282225668696	-0.101004526161372
C	2.838218287953794	1.119007847994998	-0.042604410977828
C	4.216923955351552	-0.668923032880038	-0.093781639956882
C	2.831939760279634	-1.081146806219731	-0.029604424649088
N	0.002442569814634	2.022817696583324	0.010264382244422
N	-0.007485627384980	-1.965065561551473	0.057140043505294
N	-1.995480424611422	0.036454504724320	0.018895579266198
N	1.989692278832684	0.021074683849362	-0.024304253009980
H	5.061544746928938	-1.353974161247933	-0.130494882428255
H	-5.069684786389782	1.408114789007604	-0.113273799296920
H	-5.076022032445966	-1.322604970848818	-0.069198079328601
H	-1.350762773835356	5.107828288563676	0.026131503106774
H	1.380789007498316	5.096066379010161	0.035006563010238
H	5.069815191454902	1.378005624781480	-0.144017459171614
H	-1.382294144960202	-5.038124513653838	0.157633408002594
H	1.348989048181468	-5.046885177015545	0.133412551544900
H	-3.193022547026334	3.241747667676606	-0.001955873476136
H	3.206041441860560	3.216747989567408	0.000181806851998
H	-3.210389689200770	-3.159795832996011	0.097451329344978
H	3.188107834491100	-3.180231483499270	0.040313105896892
H	-1.512453733301211	-0.054772761486474	2.915401164658356
O	0.165362631770288	0.126164140350488	2.046691231456378
O	-0.759713023668912	-0.674688745222269	2.784180051056968

Transition Metal: Co; Functional Group: NH2; Adsorbate: Clean

Co	0.028080940350878	-0.026537708603112	-0.031634825750839
C	0.810437463642112	4.075899450030512	-0.666090887701792
C	1.181553479151552	2.681097950254828	-0.611274708164039
C	2.492878002367000	2.171941752765426	-0.774788006116157
C	-0.724526734740255	-4.151650046353407	-0.484911248799524
C	-1.117613728578505	-2.763180688701656	-0.444657215718564
C	-2.409102972768604	-2.261887152529198	-0.666975862108941
C	0.591946412893924	-4.211303031378598	-0.056959202506231
C	0.989731379831790	-2.856286657796801	0.261471274397972
C	-0.460998524695356	4.175000402572461	-0.120754099086014
C	2.263778774511868	-2.466665577541733	0.729522227970650
C	-4.089165187679079	0.723022960901620	0.553894914683824
C	-0.916146218274108	2.830097153260176	0.145848140868508
C	-2.707661372540645	1.141475889405324	0.447035321305972
C	-4.151441883217295	-0.590332824163625	0.113897715141086
C	-2.801907616424970	-0.979949903407032	-0.214407049775005
C	-2.238760229542905	2.475962186367108	0.506412559400686
C	4.205315046898122	0.540024716216348	0.137822075756486
C	2.863092260691070	0.904895509835314	-0.284573105118579
C	4.111947434672288	-0.713639665891144	0.720359184568798
C	2.738828562063088	-1.150108737101398	0.570751048491098
N	0.113121264135598	1.929131727628154	-0.133759989803377
N	-0.055155016482772	-1.978140522185473	0.009760951339398
N	-1.923719970850964	0.064029025199426	0.046649068416676
N	1.978110087785814	-0.122720677944372	0.013811903807624
N	5.194342299720613	-1.479216901721209	1.286509345248264
N	-5.198265988205158	1.536241192033358	0.967917074061624
N	-5.322199158486765	-1.376849012703559	0.017980044814466
N	-1.187802165968801	5.379178507017520	0.063989843592412
N	1.649710172752188	5.165160471607843	-1.105234812240433
N	5.374731533460299	1.298323448645620	0.001213454884192
N	-1.508790672017010	-5.269992433933790	-0.884466360192572
N	1.355487358998346	-5.399817097617735	0.035929401189822
N	-3.144205366167604	3.494873550889032	0.856229874775230
N	3.526852496558958	3.016400960598202	-1.268915271745254
N	-3.401766083806780	-3.107369976977566	-1.243242386240727
N	3.129187294870574	-3.491390796005614	1.211417470408716
H	-2.455583149494522	-5.229727840980162	-0.497039932699465
H	-1.077691301743513	-6.136702840500632	-0.551001089340044
H	-2.991952965082380	-3.804813934462807	-1.866887285298201
H	-4.100378333725494	-2.571436969128598	-1.760495023757041
H	-5.357393495902249	1.509327369422184	1.980502485343050
H	-6.065336269751157	1.264988058772118	0.498702833773348
H	-1.510510172553239	5.498013817600932	1.028215578249288
H	1.238007804171548	5.669172585307354	-1.896125929384024
H	1.826749286666668	5.846321405872020	-0.359270949814402
H	3.164642886999406	3.947664934529398	-1.506064293836303
H	4.025332986294014	2.599028249408306	-2.057114252425873
H	5.175234784888980	2.286995912645566	-0.179464181784589
H	6.032955383372078	1.166206600152784	0.770640569161356
H	6.044284218799586	-1.393538716039188	0.720732038587452
H	5.427348504754864	-1.173508677694414	2.237673844104294
H	4.062435026977064	-3.115114573738623	1.419460559476686
H	2.743367261453402	-3.968691516896822	2.029234435945488
H	2.339013313523680	-5.176998525012195	0.223389481676632
H	1.291185662743632	-5.959347980057732	-0.818510261807532
H	-5.135426938763171	-2.377501414892773	0.110136372300976
H	-6.024985181394962	-1.096459372604798	0.705574007758784
H	-4.117252172146840	3.167177149664394	0.830487662021418
H	-3.012547261645928	4.351040916914522	0.314579594984320
H	-0.621145112469982	6.191283436027394	-0.192989343230593

Transition Metal: Co; Functional Group: NH2; Adsorbate: O

Co	0.030287473773718	0.005554567715906	0.508384752201248
C	0.871233824411858	4.150780380788980	-0.719658130523875
C	1.230831373733880	2.764995303562004	-0.504225922842657
C	2.560916665017356	2.249138237185270	-0.459474329992680
C	-0.788126954990055	-4.170478649692313	-0.634962222327328
C	-1.183276228616414	-2.820573336365243	-0.291026363613508
C	-2.516104543272327	-2.331800775694791	-0.182917662899150
C	0.584806385815298	-4.245952976707857	-0.435813713901403
C	1.005157007500616	-2.931144198061723	0.009241657532652
C	-0.485885947100360	4.253094842086788	-0.448373133043820
C	2.332693023816586	-2.566317486188996	0.373826069065420
C	-4.135968642918646	0.833292901267356	0.610710238936174
C	-0.954586691839182	2.912633194575810	-0.159452922999513
C	-2.776032028800710	1.217375366122684	0.300790914224516
C	-4.188177706692555	-0.551507861166716	0.539734306640260
C	-2.864078121489346	-0.995181627186522	0.159263128880744
C	-2.310654613671531	2.549780766938868	0.101741814551208
C	4.227427018627100	0.548966850329524	0.446842236049734
C	2.912451266911226	0.941839738120408	-0.024835649798597
C	4.153382446517816	-0.806980171896551	0.736610432239512
C	2.808284187788448	-1.228902865803956	0.418027431142656
N	0.108680915254038	2.031217214039448	-0.181167156478168
N	-0.075060074346709	-2.074583470239261	0.048606441661052
N	-2.003510408267534	0.090174759470716	0.078546760707898
N	2.051967130705514	-0.143596717250063	0.003534117168812
N	5.217305356621946	-1.638237402851566	1.245581035409362
N	-5.241261956042933	1.710667596910706	0.877806518448510
N	-5.338644494460521	-1.337857687024680	0.775105975098366
N	-1.250769440469615	5.448792793867908	-0.494239359332415
N	1.761553823646590	5.228826396122393	-1.086360995267537
N	5.376801313973468	1.349397175641684	0.583577959238232
N	-1.653673026896815	-5.236399714675962	-1.084404214324525
N	1.376776069575710	-5.394920590036701	-0.617927933707087
N	-3.254289256346425	3.573256235237580	0.158618013600824
N	3.610739469500572	3.127057494825580	-0.745208351068733
N	-3.554905467858099	-3.249125038472091	-0.354054742339606
N	3.245536318822054	-3.601545255075521	0.598933994287820
H	-1.488288205790685	-6.100614774165471	-0.558722517800806
H	-1.519051843286363	-5.450911268746752	-2.078708228990372
H	-3.241352122861926	-4.162225192275846	-0.706528469142434
H	-4.396480894065499	-2.886967039401100	-0.798221388266484
H	-5.294104739468237	2.002525441167054	1.859428186043706
H	-6.134486920087260	1.284541053162556	0.620412704988302
H	-1.738103490235343	5.629424913021927	0.388450637202450
H	1.464667414434210	5.691945200153715	-1.950381597514962
H	1.826795522313522	5.945181658719262	-0.354940228242953
H	3.303733820169348	4.040899535995420	-1.098933594599085
H	4.403739022842886	2.716502785623982	-1.233517891643640
H	5.161740455249790	2.336197667534992	0.737988422713860
H	6.009412561182646	0.999479460680056	1.305476207982874
H	6.105849874770360	-1.445717467963863	0.773274782719474
H	5.364613829388886	-1.500101099137449	2.251548065904616
H	4.159126806159306	-3.272415314722029	0.934638304235330
H	2.875190938959386	-4.403830961961352	1.106019782103402
H	2.350661594121852	-5.182855072499395	-0.841687361318986
H	0.978392927876356	-6.042305138082554	-1.300547691798879
H	-5.106956094816852	-2.278839645890407	1.099741506572944
H	-5.969996721335587	-0.891108738423661	1.444286917055672
H	-4.226380824914834	3.246436887501640	0.166225803895024
H	-3.667966098068101	4.369091138158220	-0.450951613970886
H	-0.654109515468580	6.254314239032076	-0.701081353762898
O	0.081785375877714	0.143465515932862	2.179744912041712

Transition Metal: Co; Functional Group: NH2; Adsorbate: OH

Co	0.018906477911454	-0.014654081671711	0.162097407808420
C	0.758448569684356	4.062736555747724	-0.700327032263985
C	1.144857415412336	2.672385899556636	-0.621966331857355
C	2.462525573873570	2.175392629144630	-0.784495265895814
C	-0.727988889677992	-4.144052252286217	-0.452492010993247
C	-1.119773373298422	-2.752236512978619	-0.433113024421729
C	-2.406789202865966	-2.252144004318769	-0.685143683472177
C	0.579642462011674	-4.202106541871720	-0.007591996443143
C	0.972437974266400	-2.839342176930320	0.301461399240680
C	-0.489370638157812	4.165721581298206	-0.102404995366513
C	2.245948832916734	-2.444092991506523	0.769379857010166
C	-4.102133980608027	0.722721183805508	0.541725887486264
C	-0.919174855727004	2.823228231059190	0.213797498834308
C	-2.717578420279800	1.131873430432024	0.471052148754124
C	-4.164678514190536	-0.576930120332801	0.059641750616544
C	-2.809824998184013	-0.963931104157044	-0.254984175247095
C	-2.235122084354348	2.456842991880190	0.609077611298568
C	4.196015987031696	0.548430997778332	0.105062731401556
C	2.848877299219034	0.911251121543470	-0.295476961843516
C	4.113242161565703	-0.709412940373245	0.684393503020334
C	2.739061630730422	-1.140236586405667	0.559804189428604
N	0.092116074179180	1.924953496530522	-0.100124031034419
N	-0.058302998036780	-1.964172941566787	0.012839458218656
N	-1.937353592515379	0.076254992279660	0.0273067455763134
N	1.971252993334492	-0.126477861438389	-0.000939831000658
N	5.199435354650134	-1.478434853688412	1.239919242138318
N	-5.212069652472366	1.532367277001734	0.964606267542572
N	-5.338305106921464	-1.350711272761732	-0.078082906515626
N	-1.239899857949698	5.364355322209001	0.077200949261354
N	1.566526327631934	5.140508071043321	-1.217239673121860
N	5.365277504230898	1.303617479613302	-0.055794904847184
N	-1.519923032872580	-5.257775713577127	-0.867497964567427
N	1.354184005219320	-5.385778292428153	0.089068085489706
N	-3.113140555048272	3.446715685028420	1.038836767831646
N	3.478643648929300	3.029938376077510	-1.274245432677397
N	-3.387574647732016	-3.098688730483758	-1.263164644334097
N	3.094719548544718	-3.448881713146619	1.292855851403604
H	-2.426997017752818	-5.268340896270114	-0.390383241730184
H	-1.047240901896647	-6.129962235242081	-0.614781747432712
H	-2.975706037198961	-3.859238563560872	-1.807042286408610
H	-4.054271885161985	-2.580785573498488	-1.837001724502432
H	-5.429704509123138	1.414018948570424	1.959976538850286
H	-6.057809149335123	1.327757414092542	0.426682174563008
H	-1.324649946087820	5.620238200974800	1.066386005043368
H	1.190582807815872	5.513822993500294	-2.094337677015986
H	1.638314526055916	5.919029233617058	-0.554568373954481
H	3.113099123807680	3.953090969993932	-1.534483260800766
H	4.040002359462590	2.606599978770164	-2.013837956958980
H	5.176611955533664	2.303428323340872	-0.163840931066584
H	6.062838001143493	1.119500917936640	0.666430312629254
H	6.018696976204150	-1.471662544337850	0.624297279976540
H	5.498380042399872	-1.117059964403374	2.152103009820598
H	4.024710746636832	-3.078002689399870	1.520948875802432
H	2.679352420567874	-3.946016557853678	2.082150783671216
H	2.333389520863084	-5.157281519110665	0.287192797893712
H	1.311884047500268	-5.938721457294957	-0.770972994954921
H	-5.160450714484144	-2.354631376451625	-0.005123152349858
H	-6.053258591893439	-1.077538825586558	0.599761616548420
H	-4.096011010992395	3.151415651839664	1.008033565822890
H	-2.937456472198182	4.367007118273216	0.631564688004526
H	-0.797801294352688	6.148502526855641	-0.409833847668928
H	0.705288240993236	0.691363836108856	2.283154259822678
O	0.005349461921980	0.051545598563768	2.048515414486646

Transition Metal: Co; Functional Group: NH2; Adsorbate: OOH

Co	0.021085337479000	-0.019437146786917	0.191367195485256
C	0.755737110467684	4.059402916069340	-0.713395482083438
C	1.139987502646070	2.668295487683958	-0.624806379101933
C	2.458226763832572	2.169631950755692	-0.781531704678915
C	-0.727266465407354	-4.142093260707174	-0.448598544634681
C	-1.117371572941916	-2.749726433895550	-0.414087685039771
C	-2.404358056579603	-2.247720938894396	-0.659461701843234
C	0.584296936652654	-4.205499114951387	-0.017707912724561
C	0.982416287191790	-2.845619381070602	0.298560494232770
C	-0.488673488140279	4.167794517667436	-0.110204780907260
C	2.261022162235320	-2.454978007021154	0.756026707593298
C	-4.102684394029181	0.730901647609356	0.566640507700354
C	-0.917824904184947	2.827450883327686	0.216806678252580
C	-2.717425645618668	1.141313074625508	0.496412949654506
C	-4.163351455919608	-0.571058626563342	0.085357938622782
C	-2.809001315374640	-0.958975726686489	-0.227643108754844
C	-2.230751465862436	2.467073587365304	0.625982312252290
C	4.196449703197080	0.549240464326082	0.107942725312996
C	2.846058877064478	0.907711566339332	-0.288459067611239
C	4.120520583202948	-0.713255443628917	0.676530891094516
C	2.748069518773636	-1.148254610035618	0.552454740449178
N	0.090349828086312	1.927209744939770	-0.095963647060657
N	-0.050607548599523	-1.967688807727754	0.030242483596190
N	-1.937320756701922	0.081434371330310	0.054572251465676
N	1.975119362900362	-0.134068317983157	0.002161902495104
N	5.210888876051940	-1.481109085580204	1.224022285652718
N	-5.218655697638852	1.549298050138802	0.959486215730026
N	-5.337413593989560	-1.340993959654334	-0.060708517530074
N	-1.239270190757683	5.367210020283774	0.068351267299560
N	1.563854787279802	5.133198959312454	-1.238088843335262
N	5.362177500520964	1.311432040458784	-0.044779788486768
N	-1.525525606280034	-5.251544769995833	-0.862565436192813
N	1.357596395545356	-5.390295211044865	0.062606059127340
N	-3.105021296924960	3.459172565621506	1.062545863978734
N	3.474128368534288	3.020358237097948	-1.276825978160552
N	-3.387772839619732	-3.089968573896073	-1.243451072473036
N	3.114982907393478	-3.464642948277920	1.264456892001456
H	-2.427894059352937	-5.261681272234981	-0.376272047162018
H	-1.052150113938911	-6.125960818194718	-0.618349777352080
H	-2.974902219337821	-3.852070990350128	-1.785155753929512
H	-4.041227236621683	-2.566134067323329	-1.827366983897466
H	-5.472472045074856	1.431359163107604	1.946080572439100
H	-6.048569617266109	1.353318952968386	0.393556675237754
H	-1.295255638391154	5.639235268102905	1.055372998207886
H	1.190772163035238	5.498092956267756	-2.119837017805786
H	1.631787820196160	5.917405272624372	-0.581776748480689
H	3.109738623714852	3.941879776891008	-1.543811236212239
H	4.037439321558288	2.590962046705294	-2.011377789122623
H	5.167406950943052	2.310081825356582	-0.153650840626540
H	6.053857538811924	1.131545834454558	0.684282392646022
H	6.036397657640844	-1.446217339031620	0.617668878839794
H	5.493842351876316	-1.137233687964279	2.148193670577644
H	4.048317355404862	-3.094247790914480	1.480040498750082
H	2.711282538886616	-3.956528680637049	2.063470430175240
H	2.337705322088782	-5.165575277207637	0.261312647210552
H	1.311408069139426	-5.933728089580745	-0.803151063016006
H	-5.162269852052017	-2.346419565973829	-0.005613110502569
H	-6.055371927809448	-1.075106287439684	0.616424481154722
H	-4.089185499367979	3.169149314726898	1.023077611574922
H	-2.923098021532752	4.379085205783836	0.655479212870408
H	-0.811351948060867	6.143712333809658	-0.442926285033348
H	-1.592566315073771	-0.200218378597722	2.837702824654002
O	0.102290754665190	0.194046035564108	2.066312818249540
O	-0.745788175801032	-0.698844122961514	2.826699616773314

Transition Metal: Co; Functional Group: OH; Adsorbate: Clean

H	9.359200000000000	16.802720000000001	8.084840000000000
H	8.023410000000000	15.181770000000000	6.970730000000000
H	12.339589999999999	5.428830000000000	6.373250000000000
H	14.013249999999999	6.808910000000000	7.259030000000000
H	10.122339999999999	4.905800000000000	7.997970000000000
H	11.979680000000000	17.095559999999999	7.618570000000000
H	6.786110000000000	8.016800000000000	8.681469999999999
H	17.079210000000000	11.990209999999999	8.346970000000001
H	16.043209999999998	8.659599999999999	7.561550000000000
H	15.206610000000000	14.030360000000000	8.675570000000000
H	5.959120000000000	13.327140000000000	7.300940000000000
H	4.915060000000000	10.024340000000000	8.206080000000000
C	10.335509999999999	15.190680000000000	7.558560000000000
C	9.930780000000000	13.814190000000000	7.542900000000000
C	8.613840000000000	13.377969999999999	7.369160000000000
C	11.645970000000000	6.837650000000000	7.539520000000000
C	12.066340000000000	8.210179999999999	7.566550000000000
C	13.394439999999999	8.635350000000001	7.472140000000000
C	10.324840000000000	6.794330000000000	7.920540000000000
C	9.909200000000000	8.169490000000000	8.090260000000001
C	11.669169999999999	15.235020000000000	7.892900000000000
C	8.594200000000001	8.595290000000000	8.335780000000000
C	15.177289999999999	11.663770000000000	8.220860000000000
C	12.087339999999999	13.861649999999999	8.068339999999999
C	13.808690000000000	12.104450000000000	8.199050000000000
C	15.192810000000000	10.329070000000000	7.892180000000000
C	13.816200000000000	9.942460000000001	7.717190000000000
C	13.402220000000000	13.441020000000000	8.326029999999999
C	6.807440000000000	11.680709999999999	7.742480000000000
C	8.187630000000000	12.072480000000001	7.615290000000000
C	6.818190000000000	10.361190000000001	8.129370000000000
C	8.189100000000000	9.929449999999999	8.173260000000001
Co	11.000750000000000	11.013450000000001	7.883160000000000
O	9.501790000000000	16.289570000000001	7.265410000000000
O	7.616540000000000	14.286460000000000	7.022890000000000
O	12.475949999999999	5.721650000000000	7.295560000000000
O	14.406549999999999	7.710550000000000	7.216340000000000
O	9.537710000000001	5.685050000000000	8.075650000000000
O	12.461530000000000	16.346950000000000	8.020780000000000
O	7.682880000000000	7.621690000000000	8.659630000000000
O	16.254970000000000	12.491479999999999	8.490900000000000
O	16.330939999999998	9.570410000000001	7.787520000000000
O	14.309160000000000	14.422599999999999	8.639820000000000
O	5.670550000000000	12.430059999999999	7.573970000000000
O	5.737240000000000	9.539780000000000	8.407220000000001
N	11.012359999999999	12.995799999999999	7.849190000000000
N	10.987240000000000	9.031820000000000	7.871280000000000
N	12.966360000000000	11.029920000000001	7.906990000000000
N	9.035460000000000	10.999280000000001	7.876230000000000

Transition Metal: Co; Functional Group: OH; Adsorbate: O

H	9.372120000000001	16.812280000000001	7.384940000000000
H	8.027810000000001	15.184310000000000	6.304720000000000
H	12.335929999999999	5.443670000000000	5.656520000000000
H	14.000760000000000	6.807480000000000	6.568190000000000
H	10.102589999999999	4.903350000000000	7.267880000000000
H	11.998699999999999	17.088880000000000	6.888270000000000
H	6.798640000000000	8.029389999999999	8.038869999999999
H	17.075489999999999	11.986960000000000	7.677590000000000
H	16.047380000000000	8.657760000000000	6.857320000000000
H	15.196470000000000	14.016060000000000	8.020940000000000
H	5.956980000000000	13.328680000000000	6.607140000000000
H	4.917720000000000	10.022600000000001	7.518520000000000
C	10.333880000000001	15.191190000000001	6.872390000000000
C	9.932359999999999	13.813910000000000	6.854210000000000
C	8.617130000000000	13.374100000000000	6.668860000000000
C	11.645360000000000	6.836870000000000	6.844360000000000
C	12.062840000000000	8.210630000000000	6.866170000000000
C	13.390450000000000	8.638270000000000	6.757760000000000
C	10.325600000000000	6.791940000000000	7.234120000000000
C	9.914940000000000	8.167650000000000	7.410130000000000
C	11.669230000000001	15.236990000000000	7.202850000000000
C	8.599600000000001	8.598560000000001	7.654630000000000
C	15.175860000000000	11.663440000000000	7.502380000000000
C	12.084360000000000	13.862880000000001	7.377460000000000
C	13.809300000000000	12.106019999999999	7.463270000000000
C	15.192280000000000	10.330710000000000	7.166760000000000
C	13.815270000000000	9.950180000000000	6.971250000000000
C	13.399570000000001	13.437189999999999	7.630920000000000
C	6.809590000000000	11.676980000000000	7.027200000000000
C	8.191380000000001	12.061940000000000	6.880050000000000
C	6.820440000000000	10.358969999999999	7.417580000000000
C	8.190289999999999	9.924490000000000	7.445480000000000
Co	11.000480000000000	11.015590000000000	7.376860000000000
O	10.991660000000000	11.032660000000000	9.106249999999999
O	9.499140000000001	16.285959999999999	6.571370000000000
O	7.621470000000000	14.287200000000000	6.348380000000000
O	12.473480000000000	5.724970000000000	6.582300000000000
O	14.397560000000000	7.708690000000000	6.524860000000000
O	9.530120000000000	5.688270000000000	7.373070000000000
O	12.468340000000000	16.344619999999999	7.312480000000000
O	7.697440000000000	7.637330000000000	8.016069999999999
O	16.247879999999999	12.490480000000000	7.790260000000000
O	16.330079999999999	9.572110000000000	7.072180000000000
O	14.298349999999999	14.407800000000000	7.976870000000000
O	5.672550000000000	12.424780000000000	6.859510000000000
O	5.743360000000000	9.535190000000000	7.697000000000000
N	11.016780000000001	13.001609999999999	7.147960000000000
N	10.983790000000001	9.025119999999999	7.171720000000000
N	12.971850000000000	11.045430000000000	7.123010000000000
N	9.033620000000001	10.978190000000000	7.101090000000000

Transition Metal: Co; Functional Group: OH; Adsorbate: OH

H	11.325270000000000	10.204250000000000	9.379830000000000
H	9.384729999999999	16.809170000000002	7.261720000000000
H	8.030300000000000	15.183680000000001	6.188010000000000
H	12.317410000000001	5.416050000000000	5.586940000000000
H	13.991479999999999	6.799170000000000	6.455480000000000
H	10.101749999999999	4.907610000000000	7.215950000000000
H	12.006880000000001	17.076570000000000	6.795980000000000
H	6.787620000000000	8.037110000000000	7.928930000000000
H	17.070499999999999	11.987100000000000	7.580890000000000
H	16.048719999999999	8.655760000000001	6.729020000000000
H	15.175689999999999	13.991759999999999	7.981620000000000
H	5.949960000000000	13.335330000000001	6.505950000000000
H	4.903840000000000	10.029430000000000	7.426310000000000
C	10.338450000000000	15.182190000000000	6.749200000000000
C	9.933070000000001	13.806089999999999	6.722780000000000
C	8.612959999999999	13.372740000000000	6.556430000000000
C	11.634650000000001	6.836360000000000	6.747670000000000
C	12.055550000000000	8.207979999999999	6.756130000000000
C	13.385690000000000	8.630789999999999	6.652640000000000
C	10.315239999999999	6.796630000000000	7.139580000000000
C	9.903729999999999	8.172450000000000	7.301170000000000
C	11.669980000000001	15.222600000000000	7.093840000000000
C	8.588509999999999	8.605820000000000	7.546750000000000
C	15.171450000000000	11.649889999999999	7.420360000000000
C	12.079340000000000	13.846740000000000	7.265790000000000
C	13.800230000000001	12.086560000000000	7.392520000000000
C	15.192190000000000	10.323010000000000	7.068730000000000
C	13.813380000000000	9.939200000000000	6.879590000000000
C	13.387169999999999	13.417610000000000	7.552340000000000
C	6.797030000000000	11.681850000000001	6.928990000000000
C	8.181940000000001	12.065500000000000	6.786210000000000
C	6.806740000000000	10.364960000000000	7.315910000000000
C	8.179460000000001	9.932570000000000	7.348060000000000
Co	10.994470000000000	11.007140000000000	7.216930000000000
O	10.974330000000000	11.068130000000000	9.086990000000000
O	9.507660000000000	16.280480000000001	6.448990000000000
O	7.619480000000000	14.289059999999999	6.239080000000000
O	12.462759999999999	5.719410000000000	6.504540000000000
O	14.390359999999999	7.699320000000000	6.414100000000000
O	9.523999999999999	5.691360000000000	7.298790000000000
O	12.469310000000000	16.329480000000000	7.222910000000000
O	7.685430000000000	7.642540000000000	7.902860000000000
O	16.240459999999999	12.482030000000000	7.710760000000000
O	16.331930000000000	9.567030000000001	6.954610000000000
O	14.279650000000000	14.386049999999999	7.919090000000000
O	5.661360000000000	12.432530000000000	6.756690000000000
O	5.729550000000000	9.536650000000000	7.587960000000000
N	11.014469999999999	12.985980000000000	7.013680000000000
N	10.975260000000000	9.032900000000000	7.052380000000000
N	12.963770000000000	11.026570000000000	7.055700000000000
N	9.025359999999999	10.986340000000000	7.017770000000000

Transition Metal: Co; Functional Group: OH; Adsorbate: OOH

H	9.369890000000000	16.803010000000000	7.145560000000000
H	8.019560000000000	15.179060000000000	6.063010000000000
H	12.338559999999999	5.426910000000000	5.415380000000000
H	13.994700000000000	6.797030000000000	6.338470000000000
H	10.105380000000000	4.897560000000000	7.017050000000000
H	11.987170000000001	17.085609999999999	6.664730000000000
H	6.780160000000000	8.006050000000000	7.719380000000000
H	17.074829999999999	11.994300000000001	7.422240000000000
H	16.049040000000002	8.650969999999999	6.625590000000000
H	15.184530000000001	14.003940000000000	7.792370000000000
H	5.946110000000000	13.322590000000000	6.356950000000000
H	4.898200000000000	9.993130000000001	7.207640000000000
H	9.498379999999999	10.593070000000001	9.844250000000001
C	10.329499999999999	15.183199999999999	6.618150000000000
C	9.927640000000000	13.805690000000000	6.593290000000000
C	8.606280000000000	13.369890000000000	6.439690000000000
C	11.639699999999999	6.832320000000000	6.583640000000000
C	12.056800000000001	8.206030000000000	6.612460000000000
C	13.388330000000000	8.628729999999999	6.534200000000000
C	10.314780000000001	6.786700000000000	6.951430000000000
C	9.900370000000001	8.161930000000000	7.119820000000000
C	11.665020000000000	15.226749999999999	6.947110000000000
C	8.585390000000000	8.587859999999999	7.376520000000000
C	15.175430000000000	11.655210000000000	7.273340000000000
C	12.080439999999999	13.851500000000000	7.110410000000000
C	13.803670000000000	12.090890000000000	7.242630000000000
C	15.194440000000000	10.323330000000000	6.942130000000000
C	13.814340000000000	9.938290000000000	6.760100000000000
C	13.391629999999999	13.424450000000000	7.387240000000000
C	6.791930000000000	11.672800000000001	6.795160000000000
C	8.176810000000000	12.062600000000000	6.672410000000000
C	6.800230000000000	10.352440000000000	7.172840000000000
C	8.173579999999999	9.920780000000001	7.214310000000000
Co	10.991870000000000	11.004300000000001	7.100150000000000
O	9.493570000000000	16.280809999999999	6.328800000000000
O	7.608680000000000	14.285480000000000	6.127010000000000
O	12.471730000000001	5.718950000000000	6.338500000000000
O	14.396300000000000	7.696790000000000	6.314540000000000
O	9.522700000000000	5.678850000000000	7.088370000000000
O	12.461150000000000	16.335819999999998	7.074010000000000
O	7.679630000000000	7.615000000000000	7.702100000000000
O	16.245680000000000	12.492839999999999	7.544090000000000
O	16.333700000000000	9.566890000000001	6.830200000000000
O	14.287900000000000	14.397650000000001	7.732650000000000
O	5.655970000000000	12.420019999999999	6.607460000000000
O	5.721600000000000	9.519700000000000	7.428550000000000
O	11.080390000000000	11.192299999999999	8.973549999999999
O	10.384200000000000	10.183719999999999	9.725630000000001
N	11.014460000000000	12.988379999999999	6.868720000000000
N	10.971769999999999	9.024860000000000	6.897170000000000
N	12.966870000000000	11.026009999999999	6.925240000000000
N	9.020730000000000	10.984190000000000	6.916840000000000

Transition Metal: Cr; Functional Group: BH2; Adsorbate: Clean

N	10.746680000000000	13.046519999999999	7.286050000000000
N	10.945270000000000	8.945449999999999	7.299800000000000
N	12.887639999999999	11.103370000000000	7.307560000000000
N	8.867860000000000	10.967340000000000	7.330940000000000
Cr	10.868570000000000	11.012869999999999	7.305700000000000
C	10.142630000000000	15.316890000000001	7.123040000000000
C	9.664310000000000	13.920520000000000	7.217510000000000
C	8.326570000000000	13.440099999999999	7.290170000000000
C	11.589900000000000	6.680740000000000	7.183850000000000
C	12.052099999999999	8.086650000000001	7.226470000000000
C	13.363899999999999	8.588530000000000	7.270870000000000
C	10.191420000000001	6.731840000000000	7.298200000000000
C	9.836810000000000	8.136540000000000	7.341390000000000
C	11.543790000000000	15.226100000000001	7.184090000000000
C	8.474150000000000	8.538600000000001	7.412290000000000
C	15.156940000000001	11.723490000000000	7.453020000000000
C	11.883360000000000	13.834720000000001	7.263030000000000
C	13.756580000000000	12.196890000000000	7.375800000000000
C	15.072030000000000	10.325329999999999	7.380460000000000
C	13.675940000000001	9.977160000000000	7.316160000000000
C	13.263900000000000	13.515829999999999	7.312150000000000
C	6.639140000000000	11.670370000000000	7.432370000000000
C	8.031510000000001	12.070959999999999	7.345540000000000
C	6.620650000000000	10.277680000000000	7.465940000000000
C	8.035729999999999	9.883950000000000	7.400660000000000
B	9.414840000000000	16.629799999999999	6.771820000000000
B	6.938230000000000	14.244009999999999	7.381220000000000
B	12.303369999999999	5.365030000000000	6.826870000000000
B	14.737240000000000	7.767080000000000	7.345820000000000
B	9.106040000000000	5.584820000000000	7.307590000000000
B	12.826330000000000	16.140039999999999	7.133770000000000
B	7.436410000000000	7.466090000000000	7.509270000000000
B	16.472370000000002	12.441470000000001	7.819700000000000
B	15.990959999999999	9.046920000000000	7.422760000000000
B	14.099200000000000	14.884230000000001	7.227430000000000
B	5.706600000000000	12.933109999999999	7.477360000000000
B	5.461250000000000	9.220110000000000	7.557660000000000
H	8.327470000000000	16.656900000000000	6.263920000000000
H	9.996409999999999	17.669920000000001	6.948260000000000
H	6.194550000000000	13.788520000000000	8.402740000000000
H	6.769970000000000	15.425789999999999	7.407380000000000
H	11.710640000000000	4.332930000000000	7.025670000000000
H	13.378010000000000	5.312990000000000	6.294890000000000
H	14.884810000000000	6.583590000000000	7.371000000000000
H	15.621070000000000	8.211760000000000	6.432870000000000
H	8.961449999999999	4.912650000000000	8.301679999999999
H	8.732120000000000	5.108820000000000	6.261620000000000
H	13.672910000000000	15.647370000000000	6.207340000000000
H	12.916729999999999	17.330230000000000	7.055120000000000
H	6.219530000000000	7.676600000000000	7.558600000000000
H	7.672660000000000	6.249120000000000	7.584040000000000
H	16.499210000000001	13.487740000000001	8.408080000000000
H	17.513940000000002	11.887520000000000	7.577140000000000
H	15.509810000000000	8.209610000000000	8.357040000000000
H	17.182810000000000	8.962940000000000	7.489260000000000
H	13.664840000000000	15.778449999999999	8.129799999999999
H	15.285850000000000	15.014989999999999	7.208840000000000
H	4.513950000000000	13.008039999999999	7.560860000000000
H	6.056520000000000	13.783010000000001	6.480590000000000
H	4.849000000000000	8.906730000000000	6.564320000000000
H	4.959040000000000	8.967680000000000	8.627260000000000

Transition Metal: Cr; Functional Group: BH2; Adsorbate: O

C	10.150150000000000	15.285480000000000	6.734920000000000
C	9.673360000000000	13.896210000000000	6.859880000000000
C	8.342350000000000	13.432940000000000	6.894150000000000
C	11.578609999999999	6.713870000000000	6.834450000000000
C	12.036190000000000	8.116600000000000	6.887950000000000
C	13.347410000000000	8.598770000000000	6.871010000000000
C	10.187550000000000	6.757850000000000	6.998780000000000
C	9.839990000000000	8.161120000000000	7.078250000000000
C	11.543030000000000	15.204940000000001	6.869850000000000
C	8.483260000000000	8.543889999999999	7.164960000000000
C	15.123220000000000	11.720660000000001	7.112310000000000
C	11.879700000000000	13.817100000000000	7.014230000000000
C	13.725700000000000	12.187400000000000	7.109190000000000
C	15.037350000000000	10.329029999999999	6.950200000000000
C	13.646839999999999	9.981909999999999	6.929080000000000
C	13.254750000000000	13.510149999999999	7.079100000000000
C	6.679050000000000	11.663919999999999	7.033440000000000
C	8.066910000000000	12.063359999999999	6.970690000000000
C	6.663200000000000	10.271170000000000	7.110950000000000
C	8.071590000000000	9.888230000000000	7.094520000000000
B	9.428080000000000	16.584949999999999	6.316140000000000
B	6.952310000000000	14.235230000000000	6.918520000000000
B	12.281499999999999	5.408960000000000	6.414030000000000
B	14.721439999999999	7.772820000000000	6.864980000000000
B	9.082150000000000	5.628080000000000	6.986520000000000
B	12.823800000000000	16.120930000000001	6.815190000000000
B	7.449480000000000	7.473140000000000	7.279930000000000
B	16.438189999999999	12.428330000000001	7.498420000000000
B	15.964359999999999	9.056970000000000	6.919870000000000
B	14.093719999999999	14.870649999999999	6.966500000000000
B	5.734850000000000	12.917940000000000	7.014850000000000
B	5.508840000000000	9.204810000000000	7.191850000000000
H	8.373810000000001	16.592770000000002	5.743850000000000
H	9.988730000000000	17.631390000000000	6.516290000000000
H	6.185300000000000	13.805619999999999	7.930570000000000
H	6.780140000000000	15.416370000000001	6.902240000000000
H	11.725890000000000	4.369500000000000	6.669310000000000
H	13.301460000000001	5.375310000000000	5.783040000000000
H	14.866190000000000	6.588830000000000	6.856430000000000
H	15.559970000000000	8.236929999999999	5.925820000000000
H	8.985720000000001	4.884340000000000	7.934350000000000
H	8.668030000000000	5.220740000000000	5.926500000000000
H	13.684010000000001	15.607630000000000	5.916720000000000
H	12.908080000000000	17.308199999999999	6.704520000000000
H	6.229650000000000	7.678130000000000	7.308300000000000
H	7.691630000000000	6.259090000000000	7.406040000000000
H	16.465640000000000	13.442900000000000	8.138310000000001
H	17.478510000000000	11.890960000000000	7.216800000000000
H	15.532480000000000	8.187170000000000	7.852840000000000
H	17.157550000000001	8.983480000000000	6.932710000000000
H	13.642720000000001	15.790050000000001	7.834770000000000
H	15.280210000000000	15.001749999999999	6.962430000000000
H	4.540600000000000	12.977119999999999	7.065380000000000
H	6.101050000000000	13.745520000000001	6.005220000000000
H	4.940600000000000	8.857049999999999	6.184140000000000
H	4.945600000000000	9.012650000000001	8.243160000000000
O	10.922650000000001	11.063870000000000	9.094130000000000
N	10.751970000000000	13.019660000000000	7.021050000000000
N	10.936109999999999	8.982590000000000	7.025050000000000
N	12.844860000000001	11.099230000000000	7.023140000000000
N	8.918220000000000	10.967620000000000	7.001190000000000
Cr	10.870870000000000	11.032760000000000	7.505530000000000

Transition Metal: Cr; Functional Group: BH2; Adsorbate: OH

C	10.1423400000000001	15.3031500000000000	6.6673400000000000
C	9.6647700000000001	13.9156499999999999	6.8213800000000000
C	8.3261900000000000	13.4385999999999999	6.8674000000000000
C	11.5836700000000000	6.6971100000000000	6.7421200000000000
C	12.0447600000000000	8.1000700000000001	6.8283900000000000
C	13.3572900000000001	8.5975600000000000	6.8519700000000000
C	10.1867699999999999	6.7439700000000000	6.8721700000000000
C	9.8357899999999999	8.1461500000000000	6.9624600000000000
C	11.5439100000000000	15.2176200000000000	6.7502600000000000
C	8.4744499999999999	8.5461399999999999	7.0183300000000000
C	15.1532699999999999	11.7263300000000001	6.9766600000000000
C	11.8832100000000000	13.8340500000000000	6.8951200000000000
C	13.7501500000000000	12.1988100000000000	6.9707700000000000
C	15.0646500000000000	10.3314900000000001	6.8957100000000000
C	13.6649800000000000	9.9835300000000000	6.8968800000000000
C	13.2640600000000001	13.5169099999999999	6.9267200000000000
C	6.6414100000000000	11.6682299999999999	6.9442800000000000
C	8.0362399999999999	12.0715299999999999	6.9159500000000000
C	6.6253800000000000	10.2774699999999999	6.9829500000000000
C	8.0433699999999999	9.8888500000000000	6.9807700000000000
B	9.4153199999999999	16.5949199999999998	6.2449700000000000
B	6.9351400000000000	14.2412700000000000	6.8997900000000000
B	12.2921600000000001	5.3960300000000000	6.3275100000000000
B	14.7315200000000000	7.7747400000000000	6.8653300000000000
B	9.0981600000000000	5.6012800000000000	6.8370600000000000
B	12.8250499999999999	16.1288400000000000	6.6541600000000000
B	7.4317600000000000	7.4754700000000000	7.0937000000000000
B	16.4836700000000000	12.4396600000000000	7.2982300000000000
B	15.9857900000000000	9.0538100000000000	6.8915500000000000
B	14.1004000000000000	14.8798999999999999	6.7881800000000000
B	5.7043000000000000	12.9280399999999999	6.9463700000000000
B	5.4685000000000000	9.2122899999999999	7.0216300000000000
H	10.9600600000000000	11.9133300000000000	9.4463100000000000
H	8.3320100000000000	16.5975900000000000	5.7283000000000000
H	9.9948099999999999	17.6426000000000002	6.3764200000000000
H	6.1521600000000000	13.7846700000000000	7.8902900000000000
H	6.7644900000000000	15.4227600000000000	6.9202500000000000
H	11.7082200000000001	4.3564800000000000	6.5122600000000000
H	13.3518700000000000	5.3633100000000000	5.7653100000000000
H	14.8785100000000000	6.5911900000000000	6.8820200000000000
H	15.5760299999999999	8.2212999999999999	5.9160400000000000
H	8.9587400000000001	4.8819600000000000	7.7979000000000000
H	8.7060700000000000	5.1828900000000000	5.7730700000000000
H	13.6689600000000000	15.6030700000000001	5.7423300000000000
H	12.9129799999999999	17.3154000000000000	6.5307200000000000
H	6.2134200000000000	7.6893200000000000	7.1169500000000000
H	7.6649600000000000	6.2598500000000000	7.1851000000000000
H	16.5346499999999999	13.4759400000000000	7.9020900000000000
H	17.5138900000000000	11.8881599999999999	7.0073300000000000
H	15.5457600000000000	8.2148600000000000	7.8438000000000000
H	17.1792799999999999	8.9727599999999999	6.9081400000000000
H	13.6702900000000000	15.8046900000000001	7.6585700000000000
H	15.2868900000000000	15.0097000000000000	6.7603100000000000
H	4.5094300000000000	12.9984900000000000	6.9830000000000000
H	6.0925100000000000	13.7773800000000001	5.9636000000000000
H	4.9212200000000000	8.8802200000000000	5.9969900000000000
H	4.8936500000000000	8.9868299999999999	8.0599500000000001
O	10.8922100000000000	11.0144900000000000	9.0707000000000000
N	10.7472600000000001	13.0452800000000000	6.9491200000000000
N	10.9420699999999999	8.9562899999999999	6.9459300000000000
N	12.8766300000000000	11.1075500000000000	6.9352600000000000
N	8.8775200000000001	10.9725400000000000	6.9360200000000000
Cr	10.8658400000000000	11.0231400000000000	7.2297800000000000

Transition Metal: Cr; Functional Group: BH2; Adsorbate: OOH

Cr	10.870870000000000	11.032760000000000	7.505530000000000
C	10.150150000000000	15.285480000000000	6.734920000000000
C	9.673360000000001	13.896210000000000	6.859880000000000
C	8.342350000000000	13.432940000000000	6.894150000000000
C	11.578609999999999	6.713870000000000	6.834450000000000
C	12.036190000000000	8.116600000000000	6.887950000000000
C	13.347410000000000	8.598770000000000	6.871010000000000
C	10.187550000000000	6.757850000000000	6.998780000000000
C	9.839990000000000	8.161120000000000	7.078250000000000
C	11.543030000000000	15.204940000000001	6.869850000000000
C	8.483260000000000	8.543889999999999	7.164960000000000
C	15.123220000000000	11.720660000000001	7.112310000000000
C	11.879700000000000	13.817100000000000	7.014230000000000
C	13.725700000000000	12.187400000000000	7.109190000000000
C	15.037350000000000	10.329029999999999	6.950200000000000
C	13.646839999999999	9.981909999999999	6.929080000000000
C	13.254750000000000	13.510149999999999	7.079100000000000
C	6.679050000000000	11.663919999999999	7.033440000000000
C	8.066910000000000	12.063359999999999	6.970690000000000
C	6.663200000000000	10.271170000000000	7.110950000000000
C	8.071590000000000	9.888230000000000	7.094520000000000
B	9.428080000000000	16.584949999999999	6.316140000000000
B	6.952310000000000	14.235230000000000	6.918520000000000
B	12.281499999999999	5.408960000000000	6.414030000000000
B	14.721439999999999	7.772820000000000	6.864980000000000
B	9.082150000000000	5.628080000000000	6.986520000000000
B	12.823800000000000	16.120930000000001	6.815190000000000
B	7.449480000000000	7.473140000000000	7.279930000000000
B	16.438189999999999	12.428330000000001	7.498420000000000
B	15.964359999999999	9.056970000000000	6.919870000000000
B	14.093719999999999	14.870649999999999	6.966500000000000
B	5.734850000000000	12.917940000000000	7.014850000000000
B	5.508840000000000	9.204810000000000	7.191850000000000
H	8.373810000000001	16.592770000000002	5.743850000000000
H	9.988730000000000	17.631390000000000	6.516290000000000
H	6.185300000000000	13.805619999999999	7.930570000000000
H	6.780140000000000	15.416370000000001	6.902240000000000
H	11.725890000000000	4.369500000000000	6.669310000000000
H	13.301460000000001	5.375310000000000	5.783040000000000
H	14.866190000000000	6.588830000000000	6.856430000000000
H	15.559970000000000	8.236929999999999	5.925820000000000
H	8.985720000000001	4.884340000000000	7.934350000000000
H	8.668030000000000	5.220740000000000	5.926500000000000
H	13.684010000000001	15.607630000000000	5.916720000000000
H	12.908080000000000	17.308199999999999	6.704520000000000
H	6.229650000000000	7.678130000000000	7.308300000000000
H	7.691630000000000	6.259090000000000	7.406040000000000
H	16.465640000000000	13.442900000000000	8.138310000000001
H	17.478510000000000	11.890960000000000	7.216800000000000
H	15.532480000000000	8.187170000000000	7.852840000000000
H	17.157550000000001	8.983480000000000	6.932710000000000
H	13.642720000000001	15.790050000000001	7.834770000000000
H	15.280210000000000	15.001749999999999	6.962430000000000
H	4.540600000000000	12.977119999999999	7.065380000000000
H	6.101050000000000	13.745520000000001	6.005220000000000
H	4.940600000000000	8.857049999999999	6.184140000000000
H	4.945600000000000	9.012650000000001	8.243160000000000
N	10.751970000000000	13.019660000000000	7.021050000000000
N	10.936109999999999	8.982590000000000	7.025050000000000
N	12.844860000000001	11.099230000000000	7.023140000000000
N	8.918220000000000	10.967620000000000	7.001190000000000
O	10.932462135999895	11.069765240458800	9.395164361711693
H	9.342386154979147	11.435540438160226	10.388377011637717
O	9.817572071617601	10.592327782608585	10.230576668997005

Transition Metal: Cr; Functional Group: CH3; Adsorbate: Clean

Cr	10.977580000000000	11.040749999999999	7.356090000000000
C	10.399839999999999	15.287039999999999	7.522360000000000
C	9.904410000000000	13.911910000000001	7.464210000000000
C	8.545610000000000	13.491660000000000	7.518770000000000
C	11.637449999999999	6.841940000000000	8.051869999999999
C	12.042249999999999	8.247450000000001	8.045280000000000
C	13.338550000000000	8.752879999999999	8.337809999999999
C	10.347329999999999	6.788890000000000	7.543420000000000
C	9.933059999999999	8.167400000000001	7.286260000000000
C	11.739970000000000	15.252280000000001	7.164930000000000
C	8.628060000000000	8.604240000000001	6.934620000000000
C	15.228140000000000	11.621010000000000	7.050660000000000
C	12.088720000000000	13.850800000000000	6.963390000000000
C	13.835080000000000	12.055650000000000	6.951210000000000
C	15.219130000000000	10.368720000000000	7.648980000000000
C	13.819120000000000	10.004009999999999	7.857420000000000
C	13.375000000000000	13.352880000000001	6.604930000000000
C	6.734200000000000	11.658120000000000	7.650840000000000
C	8.112539999999999	12.136520000000001	7.538770000000000
C	6.751250000000000	10.297900000000000	7.379210000000000
C	8.147140000000000	9.921680000000000	7.183030000000000
C	9.687960000000000	16.515059999999998	8.036910000000001
C	7.477680000000000	14.567950000000000	7.345990000000000
C	12.466630000000000	5.632920000000000	8.408490000000000
C	14.246810000000000	7.937910000000000	9.250299999999999
C	9.525840000000001	5.529940000000000	7.418960000000000
C	12.668270000000000	16.440329999999999	7.168680000000000
C	7.701040000000000	7.633680000000000	6.212460000000000
C	16.476459999999999	12.387630000000000	6.692510000000000
C	16.446010000000001	9.524179999999999	7.891480000000000
C	14.272090000000000	14.260439999999999	5.772420000000000
C	5.519700000000000	12.411989999999999	8.136960000000000
C	5.553070000000000	9.386030000000000	7.452950000000000
N	10.979500000000000	13.060720000000000	7.221350000000000
N	10.987080000000001	9.019860000000000	7.581280000000000
N	13.010109999999999	11.038980000000000	7.415410000000000
N	8.950329999999999	11.040220000000000	7.346380000000000
H	8.937939999999999	16.267779999999998	8.799300000000001
H	10.405889999999999	17.205210000000001	8.504799999999999
H	9.174840000000000	17.086810000000000	7.243590000000000
H	6.622540000000000	14.176489999999999	6.785540000000000
H	7.091930000000000	14.974660000000000	8.295780000000001
H	7.867700000000000	15.408340000000001	6.763210000000000
H	12.598670000000000	5.505330000000000	9.496210000000000
H	12.000159999999999	4.713650000000000	8.029410000000000
H	13.472030000000000	5.682930000000000	7.966220000000000
H	14.906060000000000	8.604720000000000	9.818870000000000
H	13.646010000000000	7.389030000000000	9.985620000000001
H	14.887460000000001	7.202600000000000	8.736700000000001
H	9.372880000000000	5.217220000000000	6.372260000000000
H	10.010100000000000	4.693310000000000	7.939790000000000
H	8.528969999999999	5.647430000000000	7.867870000000000
H	12.245210000000000	17.265190000000000	7.759350000000000
H	13.649620000000001	16.198589999999999	7.601290000000000
H	12.848560000000001	16.840579999999999	6.156230000000000
H	8.284170000000000	6.971730000000000	5.560280000000000
H	7.092230000000000	6.992010000000000	6.869650000000000
H	7.010150000000000	8.185810000000000	5.563850000000000
H	16.471399999999999	13.401230000000000	7.119470000000000
H	17.370429999999999	11.884589999999999	7.084320000000000
H	16.614950000000000	12.497859999999999	5.603810000000000
H	16.750499999999999	9.499040000000001	8.951630000000000
H	16.292639999999999	8.482570000000001	7.575530000000000
H	17.302209999999999	9.905650000000000	7.318850000000000
H	15.005470000000001	14.845860000000000	6.350330000000000
H	14.834360000000000	13.665960000000000	5.041230000000000

H	13.664000000000000	14.970440000000000	5.199700000000000
H	4.818380000000000	11.727370000000001	8.636550000000000
H	5.782100000000000	13.188950000000000	8.866650000000000
H	4.955350000000000	12.901730000000001	7.323930000000000
H	5.774280000000000	8.452120000000001	7.989880000000000
H	4.720020000000000	9.874510000000001	7.977530000000000
H	5.173350000000000	9.105020000000000	6.455900000000000

Transition Metal: Cr; Functional Group: CH3; Adsorbate: O

Cr	10.978960000000001	11.002700000000001	6.767510000000000
C	10.466150000000001	15.212300000000001	7.599060000000000
C	9.955460000000000	13.846190000000000	7.521240000000000
C	8.605890000000000	13.439760000000000	7.667350000000000
C	11.578210000000000	6.930870000000000	8.106019999999999
C	11.980630000000000	8.335500000000000	8.057330000000000
C	13.243520000000000	8.858390000000000	8.428129999999999
C	10.348800000000001	6.841220000000000	7.468350000000000
C	9.956619999999999	8.203630000000000	7.125410000000000
C	11.754870000000000	15.192190000000000	7.086220000000000
C	8.671670000000001	8.624689999999999	6.709570000000000
C	15.170349999999999	11.619410000000000	6.993730000000000
C	12.071199999999999	13.799659999999999	6.809430000000000
C	13.785349999999999	12.034190000000001	6.812350000000000
C	15.139239999999999	10.431979999999999	7.714350000000000
C	13.735120000000000	10.073779999999999	7.883260000000000
C	13.336150000000000	13.307390000000000	6.390610000000000
C	6.813710000000000	11.598929999999999	7.723760000000000
C	8.183669999999999	12.088480000000001	7.600980000000000
C	6.814390000000000	10.278829999999999	7.296410000000000
C	8.200110000000000	9.925459999999999	7.032370000000000
C	9.833119999999999	16.409179999999999	8.268649999999999
C	7.535890000000000	14.525510000000001	7.684810000000000
C	12.364129999999999	5.755330000000000	8.630210000000000
C	14.085050000000001	8.120880000000000	9.458930000000001
C	9.543229999999999	5.579120000000000	7.296610000000000
C	12.681760000000001	16.378060000000001	7.013650000000000
C	7.775390000000000	7.679940000000000	5.926400000000000
C	16.419720000000002	12.359299999999999	6.589790000000000
C	16.354710000000001	9.631150000000000	8.110450000000000
C	14.206610000000000	14.179500000000001	5.501230000000000
C	5.625300000000000	12.286880000000000	8.353610000000000
C	5.612770000000000	9.369600000000000	7.285090000000000
N	10.990539999999999	12.997080000000000	7.134220000000000
N	10.973739999999999	9.080719999999999	7.460570000000000
N	12.938050000000000	11.059419999999999	7.322260000000000
N	9.018219999999999	11.019280000000000	7.274240000000000
O	11.007999999999999	10.857310000000000	5.174690000000000
H	9.160250000000000	16.114470000000001	9.084160000000001
H	10.608630000000000	17.052900000000001	8.710440000000000
H	9.253679999999999	17.043350000000000	7.574800000000000
H	6.634260000000000	14.188560000000001	7.164470000000000
H	7.236140000000000	14.837870000000001	8.699159999999999
H	7.880490000000000	15.417420000000000	7.153620000000000
H	12.397720000000000	5.719990000000000	9.732010000000001
H	11.923750000000000	4.808370000000000	8.290720000000000
H	13.405090000000000	5.766280000000000	8.275610000000000
H	14.703640000000000	8.831670000000001	10.019909999999999
H	13.434770000000000	7.623740000000000	10.189270000000000
H	14.759209999999999	7.353410000000000	9.045059999999999
H	9.446470000000000	5.276990000000000	6.240830000000000
H	10.004519999999999	4.739940000000000	7.833790000000000
H	8.523380000000000	5.689030000000000	7.695170000000000
H	12.286160000000001	17.221180000000000	7.596860000000000
H	13.683389999999999	16.148260000000001	7.406330000000000
H	12.814050000000000	16.744219999999999	5.981640000000000
H	8.384280000000000	7.030350000000000	5.284800000000000
H	7.135550000000000	7.027340000000000	6.541930000000000
H	7.116050000000000	8.253660000000000	5.262760000000000
H	16.427050000000001	13.390900000000000	6.973660000000000
H	17.315829999999998	11.867000000000001	6.989730000000000
H	16.541440000000001	12.421189999999999	5.496150000000000
H	16.584320000000002	9.704120000000000	9.187030000000000
H	16.235779999999998	8.563620000000000	7.876520000000000
H	17.244430000000001	9.977670000000000	7.567630000000000
H	14.957640000000000	14.783049999999999	6.036020000000000

H	14.745609999999999	13.555790000000000	4.776130000000000
H	13.580310000000001	14.869600000000000	4.922900000000000
H	4.962170000000000	11.546329999999999	8.824759999999999
H	5.927090000000000	12.989770000000000	9.140470000000001
H	5.009090000000000	12.847530000000001	7.628950000000000
H	5.809830000000000	8.411220000000000	7.788810000000000
H	4.761100000000000	9.839219999999999	7.795850000000000
H	5.275390000000000	9.134930000000001	6.262060000000000

Transition Metal: Cr; Functional Group: CH3; Adsorbate: OH

Cr	10.9874100000000001	11.0254800000000000	7.0169900000000000
C	10.4451500000000000	15.2571999999999999	7.5822300000000000
C	9.9324200000000000	13.8899600000000000	7.5117100000000000
C	8.5769400000000000	13.4766499999999999	7.6220100000000000
C	11.6051300000000001	6.8914000000000000	8.0917900000000000
C	12.0213699999999999	8.2941900000000000	8.0536700000000000
C	13.3071000000000000	8.8059200000000000	8.3751200000000001
C	10.3464500000000001	6.8254300000000000	7.5100800000000000
C	9.9548500000000000	8.1956900000000001	7.1917600000000000
C	11.7550700000000000	15.2264000000000000	7.1239500000000000
C	8.6669699999999999	8.6309000000000000	6.7856200000000000
C	15.2140900000000001	11.6424500000000000	7.0430900000000000
C	12.0806900000000001	13.8296600000000001	6.8710600000000000
C	13.8214200000000000	12.0503600000000000	6.8766400000000000
C	15.1988100000000000	10.4219300000000000	7.7048400000000000
C	13.7961899999999999	10.0434699999999999	7.8728000000000000
C	13.3544699999999999	13.3283700000000000	6.4779000000000000
C	6.7739700000000000	11.6293200000000000	7.6937500000000000
C	8.1455000000000000	12.1232700000000000	7.5770100000000000
C	6.7873400000000000	10.2933500000000000	7.3167100000000000
C	8.1790299999999999	9.9369200000000001	7.0730900000000000
C	9.7879900000000001	16.4695100000000000	8.1983999999999999
C	7.5066200000000000	14.5626400000000000	7.5975700000000000
C	12.3959499999999999	5.6935800000000000	8.5556800000000001
C	14.1887000000000001	8.0170100000000001	9.3330500000000000
C	9.5178700000000000	5.5730200000000000	7.3749900000000000
C	12.6892499999999999	16.4085399999999999	7.0816100000000000
C	7.7678500000000000	7.6750400000000000	6.0153900000000000
C	16.4565100000000002	12.4207800000000001	6.6911400000000000
C	16.4286199999999999	9.6193000000000001	8.0506100000000001
C	14.2318000000000000	14.2118699999999999	5.6032300000000000
C	5.5713300000000000	12.3348499999999999	8.2751900000000000
C	5.5933800000000000	9.3737100000000001	7.3356700000000000
N	10.9843200000000000	13.0401900000000001	7.1742400000000000
N	10.9933700000000001	9.0523700000000000	7.5134500000000000
N	12.9940900000000000	11.0479000000000000	7.3571200000000000
N	8.9809300000000001	11.0456500000000000	7.2883800000000000
O	11.0255700000000000	10.8599999999999999	5.1622500000000000
H	10.3566699999999999	11.4430499999999999	4.7557800000000000
H	9.0925900000000000	16.1953900000000000	9.0022699999999999
H	10.5481000000000000	17.1295399999999999	8.6426700000000001
H	9.2268399999999999	17.0808600000000001	7.4699300000000000
H	6.6140600000000000	14.2145600000000001	7.0686200000000000
H	7.1888300000000000	14.8943700000000000	8.6003700000000000
H	7.8607300000000000	15.4448200000000000	7.0558900000000000
H	12.4681400000000000	5.6256100000000000	9.6542999999999999
H	11.9327500000000000	4.7622600000000000	8.2040700000000000
H	13.4231300000000000	5.7037900000000000	8.1639100000000000
H	14.8318300000000000	8.6978600000000000	9.9025400000000000
H	13.5693699999999999	7.4843800000000000	10.0642300000000000
H	14.8427700000000000	7.2716100000000000	8.8522200000000001
H	9.3914100000000000	5.2561900000000000	6.3266200000000000
H	9.9793699999999999	4.7354500000000000	7.9144700000000000
H	8.5098000000000000	5.7036900000000000	7.7962000000000000
H	12.2847700000000000	17.2489400000000001	7.6632600000000000
H	13.6807200000000001	16.1699100000000002	7.4944400000000000
H	12.8456200000000000	16.7829900000000002	6.0557400000000000
H	8.3773599999999999	7.0264900000000000	5.3735300000000000
H	7.1356900000000000	7.0227900000000000	6.6385900000000000
H	7.1018100000000000	8.2416699999999999	5.3526900000000000
H	16.4282499999999998	13.4423600000000001	7.0998100000000000
H	17.3522900000000000	11.9399400000000000	7.1056400000000000
H	16.6076000000000001	12.5124099999999999	5.6030900000000000
H	16.6741600000000001	9.6482100000000001	9.1259599999999999
H	16.3185199999999999	8.5617699999999999	7.7722500000000000
H	17.3058100000000001	9.9987499999999999	7.5094900000000000

H	14.973039999999999	14.817840000000000	6.148320000000000
H	14.780870000000000	13.593040000000000	4.881830000000000
H	13.607970000000000	14.900430000000000	5.020560000000000
H	4.891920000000000	11.607480000000001	8.743420000000000
H	5.853990000000000	13.054800000000000	9.054100000000000
H	4.977910000000000	12.880920000000000	7.521100000000000
H	5.804790000000000	8.427440000000001	7.856070000000000
H	4.742090000000000	9.845330000000001	7.845400000000000
H	5.248110000000000	9.115399999999999	6.320870000000000

Transition Metal: Cr; Functional Group: CH3; Adsorbate: OOH

Cr	10.978960000000001	11.002700000000001	6.767510000000000
C	10.466150000000001	15.212300000000001	7.599060000000000
C	9.955460000000000	13.846190000000000	7.521240000000000
C	8.605890000000000	13.439760000000000	7.667350000000000
C	11.578210000000000	6.930870000000000	8.106019999999999
C	11.980630000000000	8.335500000000000	8.057330000000000
C	13.243520000000000	8.858390000000000	8.428129999999999
C	10.348800000000001	6.841220000000000	7.468350000000000
C	9.956619999999999	8.203630000000000	7.125410000000000
C	11.754870000000000	15.192190000000000	7.086220000000000
C	8.671670000000001	8.624689999999999	6.709570000000000
C	15.170349999999999	11.619410000000000	6.993730000000000
C	12.071199999999999	13.799659999999999	6.809430000000000
C	13.785349999999999	12.034190000000001	6.812350000000000
C	15.139239999999999	10.431979999999999	7.714350000000000
C	13.735120000000000	10.073779999999999	7.883260000000000
C	13.336150000000000	13.307390000000000	6.390610000000000
C	6.813710000000000	11.598929999999999	7.723760000000000
C	8.183669999999999	12.088480000000001	7.600980000000000
C	6.814390000000000	10.278829999999999	7.296410000000000
C	8.200110000000000	9.925459999999999	7.032370000000000
C	9.833119999999999	16.409179999999999	8.268649999999999
C	7.535890000000000	14.525510000000001	7.684810000000000
C	12.364129999999999	5.755330000000000	8.630210000000000
C	14.085050000000001	8.120880000000000	9.458930000000001
C	9.543229999999999	5.579120000000000	7.296610000000000
C	12.681760000000001	16.378060000000001	7.013650000000000
C	7.775390000000000	7.679940000000000	5.926400000000000
C	16.419720000000002	12.359299999999999	6.589790000000000
C	16.354710000000001	9.631150000000000	8.110450000000000
C	14.206610000000000	14.179500000000001	5.501230000000000
C	5.625300000000000	12.286880000000000	8.353610000000000
C	5.612770000000000	9.369600000000000	7.285090000000000
N	10.990539999999999	12.997080000000000	7.134220000000000
N	10.973739999999999	9.080719999999999	7.460570000000000
N	12.938050000000000	11.059419999999999	7.322260000000000
N	9.018219999999999	11.019280000000000	7.274240000000000
H	9.160250000000000	16.114470000000001	9.084160000000001
H	10.608630000000000	17.052900000000001	8.710440000000000
H	9.253679999999999	17.043350000000000	7.574800000000000
H	6.634260000000000	14.188560000000001	7.164470000000000
H	7.236140000000000	14.837870000000001	8.699159999999999
H	7.880490000000000	15.417420000000000	7.153620000000000
H	12.397720000000000	5.719990000000000	9.732010000000001
H	11.923750000000000	4.808370000000000	8.290720000000000
H	13.405090000000000	5.766280000000000	8.275610000000000
H	14.703640000000000	8.831670000000001	10.019909999999999
H	13.434770000000000	7.623740000000000	10.189270000000000
H	14.759209999999999	7.353410000000000	9.045059999999999
H	9.446470000000000	5.276990000000000	6.240830000000000
H	10.004519999999999	4.739940000000000	7.833790000000000
H	8.523380000000000	5.689030000000000	7.695170000000000
H	12.286160000000001	17.221180000000000	7.596860000000000
H	13.683389999999999	16.148260000000001	7.406330000000000
H	12.814050000000000	16.744219999999999	5.981640000000000
H	8.384280000000000	7.030350000000000	5.284800000000000
H	7.135550000000000	7.027340000000000	6.541930000000000
H	7.116050000000000	8.253660000000000	5.262760000000000
H	16.427050000000001	13.390900000000000	6.973660000000000
H	17.315829999999998	11.867000000000001	6.989730000000000
H	16.541440000000001	12.421189999999999	5.496150000000000
H	16.584320000000002	9.704120000000000	9.187030000000000
H	16.235779999999998	8.563620000000000	7.876520000000000
H	17.244430000000001	9.977670000000000	7.567630000000000
H	14.957640000000000	14.783049999999999	6.036020000000000
H	14.745609999999999	13.555790000000000	4.776130000000000

H	13.5803100000000001	14.8696000000000000	4.9229000000000000
H	4.9621700000000000	11.5463299999999999	8.8247599999999999
H	5.9270900000000000	12.9897700000000000	9.1404700000000001
H	5.0090900000000000	12.8475300000000001	7.6289500000000000
H	5.8098300000000000	8.4112200000000000	7.7888100000000000
H	4.7611000000000000	9.8392199999999999	7.7958500000000000
H	5.2753900000000000	9.1349300000000001	6.2620600000000000
O	11.013287972251931	10.830835541125742	4.884649092206509
H	9.665888519898251	9.804319029914200	4.001822350057872
O	9.784535828437376	10.775046021019110	4.074775149238836

Transition Metal: Cr; Functional Group: F; Adsorbate: Clean

Cr	0.000000000000000	0.000127946849674	-0.002768402677332
C	0.686444722655824	4.272685549164894	-0.002657241600559
C	1.114731036491644	2.895702771740396	-0.002502216137136
C	2.438780289494968	2.438841940090332	-0.001231768321412
C	-0.686429674745767	-4.272588458215207	-0.002687980468853
C	-1.114703932102984	-2.895608521458524	-0.002900560384170
C	-2.438747472496765	-2.438769688030003	-0.000666092840362
C	0.686429674745768	-4.272588458215207	-0.002687980468853
C	1.114703932102986	-2.895608521458524	-0.002900560384170
C	-0.686444722655818	4.272685549164894	-0.002657241600559
C	2.438747472496768	-2.438769688030003	-0.000666092840362
C	-4.272486676395548	0.686386718942832	0.002110235456394
C	-1.114731036491644	2.895702771740396	-0.002502216137136
C	-2.895495113162291	1.114750373750500	0.000474213884566
C	-4.272433696328612	-0.686464135468583	0.002100694598548
C	-2.895455693137261	-1.114725940511001	0.000752808569302
C	-2.438780289494964	2.438841940090332	-0.001231768321412
C	4.272486676395542	0.686386718942832	0.002110235456394
C	2.895495113162296	1.114750373750500	0.000474213884566
C	4.272433696328606	-0.686464135468583	0.002100694598548
C	2.895455693137258	-1.114725940511001	0.000752808569302
N	0.000000000000000	2.062746707574824	-0.003273486796862
N	0.000000000000000	-2.062611691194153	-0.003860435194802
N	-2.062516674276441	0.000019765045250	0.000254617515062
N	2.062516674276432	0.000019765045250	0.000254617515062
F	5.362227830682306	-1.474784494000925	0.000943255084568
F	-5.362516053914394	1.474415645898296	0.001029831125044
F	-5.362227830682304	-1.474784494000925	0.000943255084568
F	-1.474740934887702	5.362498928465848	-0.001737413546920
F	1.474740934887696	5.362498928465848	-0.001737413546920
F	5.362516053914396	1.474415645898296	0.001029831125044
F	-1.474773952047293	-5.362376085780376	-0.001473559681969
F	1.474773952047296	-5.362376085780376	-0.001473559681969
F	-3.403927512745597	3.403769555060228	-0.000949384290530
F	3.403927512745610	3.403769555060228	-0.000949384290530
F	-3.403900634933418	-3.403675406309063	0.000936723372662
F	3.403900634933414	-3.403675406309063	0.000936723372662

Transition Metal: Cr; Functional Group: F; Adsorbate: O

Cr	0.000000000000000	-0.001021819993447	0.465961670578424
C	0.685687296939738	4.245573332829212	-0.013363604972602
C	1.108253671362150	2.868810994240356	-0.006446191450368
C	2.432286046392846	2.428611543256712	-0.001301626763380
C	-0.685688301042763	-4.247341191762558	-0.014569887977164
C	-1.108264578543242	-2.870578037668963	-0.007546543205466
C	-2.432297884568431	-2.430347544467232	-0.002049261899986
C	0.685688301042764	-4.247341191762558	-0.014569887977164
C	1.108264578543242	-2.870578037668963	-0.007546543205466
C	-0.685687296939747	4.245573332829212	-0.013363604972602
C	2.432297884568434	-2.430347544467232	-0.002049261899986
C	-4.254415918768533	0.684711428450864	-0.014209597460649
C	-1.108253671362288	2.868810994240356	-0.006446191450368
C	-2.876799181553441	1.106371678055146	-0.000276598179475
C	-4.254437032680691	-0.686389694002777	-0.014474635390091
C	-2.876840362494939	-1.108109781341639	-0.000673662669929
C	-2.432286046392843	2.428611543256712	-0.001301626763380
C	4.254415918768536	0.684711428450864	-0.014209597460649
C	2.876799181553306	1.106371678055146	-0.000276598179475
C	4.254437032680694	-0.686389694002777	-0.014474635390091
C	2.876840362494932	-1.108109781341639	-0.000673662669929
N	0.000000000000000	2.024106614994266	-0.004832664924538
N	0.000000000000000	-2.025889124043800	-0.005889221722534
N	-2.033572679154251	-0.000882597479116	0.008255698937040
N	2.033572679154250	-0.000882597479116	0.008255698937040
F	5.340626201075152	-1.477763479012957	-0.030153300885686
F	-5.340555684631148	1.476201984707332	-0.029519072548911
F	-5.340626201075144	-1.477763479012957	-0.030153300885686
F	-1.475913913071516	5.332690521609074	-0.019156122947347
F	1.475913913071374	5.332690521609074	-0.019156122947347
F	5.340555684631154	1.476201984707332	-0.029519072548911
F	-1.475883589551387	-5.334477943107913	-0.020220196354927
F	1.475883589551390	-5.334477943107913	-0.020220196354927
F	-3.393779907495080	3.393607035766452	-0.002503840006570
F	3.393779907495072	3.393607035766452	-0.002503840006570
F	-3.393805449609474	-3.395342848656256	-0.003058744147432
F	3.393805449609474	-3.395342848656256	-0.003058744147432
O	0.000000000000000	-0.001506473788130	2.056164591913828

Transition Metal: Cr; Functional Group: F; Adsorbate: OH

Cr	0.000000000000000	0.001771992390000	0.270129700799952
C	0.686682536320642	4.266116123198758	-0.014787767746611
C	1.114744634418170	2.890486389098266	0.000688177508986
C	2.439380410170998	2.436431353240454	0.000698057926304
C	-0.686341751308724	-4.265556874879255	-0.012860678960863
C	-1.112701709106179	-2.888594955593391	-0.001764554696628
C	-2.436802758766280	-2.434792854459413	0.003666507697086
C	0.686341751308716	-4.265556874879255	-0.012860678960863
C	1.112701709106176	-2.888594955593391	-0.001764554696628
C	-0.686682536320639	4.266116123198758	-0.014787767746611
C	2.436802758766278	-2.434792854459413	0.003666507697086
C	-4.271019413286254	0.685707804088858	-0.007271696070287
C	-1.114744634418162	2.890486389098266	0.000688177508986
C	-2.892959540456744	1.113177937868444	-0.008152088763872
C	-4.269603491319703	-0.685889020884133	-0.005247631613617
C	-2.890721100712767	-1.111339422292318	-0.004667105958358
C	-2.439380410171005	2.436431353240454	0.000698057926304
C	4.271019413286248	0.685707804088858	-0.007271696070287
C	2.892959540456744	1.113177937868444	-0.008152088763872
C	4.269603491319700	-0.685889020884133	-0.005247631613617
C	2.890721100712762	-1.111339422292318	-0.004667105958358
N	0.000000000000000	2.055794760655558	0.007930797471698
N	0.000000000000000	-2.055304236246688	-0.000827868774490
N	-2.058112030073353	0.001352780869144	-0.014493630879816
N	2.058112030073358	0.001352780869144	-0.014493630879816
F	5.356598260106322	-1.476991535105881	-0.010076657769673
F	-5.359314367582563	1.475471679736618	-0.012915348055319
F	-5.356598260106320	-1.476991535105881	-0.010076657769673
F	-1.474592322712326	5.355341297165138	-0.032837930328608
F	1.474592322712318	5.355341297165138	-0.032837930328608
F	5.359314367582559	1.475471679736618	-0.012915348055319
F	-1.475096165168416	-5.354046279048141	-0.028858991464585
F	1.475096165168420	-5.354046279048141	-0.028858991464585
F	-3.402122696549789	3.401853923277204	0.001423205446602
F	3.402122696549786	3.401853923277204	0.001423205446602
F	-3.400000717843934	-3.399050981693975	0.006111885826050
F	3.400000717843932	-3.399050981693975	0.006111885826050
H	0.000000000000000	0.876102185757710	2.505671541537020
O	0.000000000000000	-0.020599431729138	2.119418324771596

Transition Metal: Cr; Functional Group: F; Adsorbate: OOH

Cr	0.001667870020656	0.031337576241868	0.292642911255458
C	0.691484890297166	4.302068394289241	-0.013239330120328
C	1.118068271266036	2.924241584623150	-0.003540071450604
C	2.442413764070022	2.470945351655412	-0.000065097550186
C	-0.680264892437428	-4.232207311586730	-0.002025934792506
C	-1.106901798975667	-2.854798175670005	0.006949888452290
C	-2.430303052516610	-2.401787231299672	0.011378673721804
C	0.691943492559890	-4.232313765505417	0.000124293558008
C	1.117746404325828	-2.854467243822953	0.009690022340678
C	-0.680687159447242	4.302269396309105	-0.010320356492248
C	2.441231878972268	-2.400711433288819	0.012978740147532
C	-4.263949278292383	0.720851127584168	-0.014762133772694
C	-1.107495493917515	2.924704683244354	0.000756958017478
C	-2.887311932435917	1.148940541693076	0.001633688036198
C	-4.262481872699173	-0.652137920323952	-0.014540352442334
C	-2.885208866890657	-1.078025235704480	0.003403822321220
C	-2.431944159950973	2.472328999811146	0.005715115899560
C	4.274091342748658	0.719412893125470	-0.013681031477269
C	2.896337943722260	1.147187973582742	-0.006763317670305
C	4.272773727049330	-0.652741026162786	-0.007791714205514
C	2.894657238438766	-1.076912563442878	0.001871281471876
N	0.005661636721588	2.090920137676484	0.000417723103942
N	0.004864353856088	-2.021341292026253	0.009986878226490
N	-2.052974544085206	0.035579219109116	0.010814357362202
N	2.062220921940612	0.035919368561394	-0.003781068175268
F	5.359752694647004	-1.443939266414027	-0.017231816808611
F	-5.354354681655554	1.507809970889000	-0.034270808726507
F	-5.350605432593982	-1.442090404263080	-0.034152740679115
F	-1.470077998836071	5.390952118092533	-0.024090319835604
F	1.479992958847036	5.390657959561111	-0.029477385116671
F	5.363414333719351	1.507264435440182	-0.028556490655220
F	-1.469593275036342	-5.320286069024508	-0.017209895006884
F	1.481606146277270	-5.320286130361234	-0.015093182254402
F	-3.396352682278469	3.436507296103218	0.003655726497786
F	3.405992253062900	3.434756212211634	0.001059341173476
F	-3.394212255176964	-3.365405578506962	0.008794369380252
F	3.404612115113278	-3.364719660942793	0.015923879078620
H	-1.441163427978577	-0.208420504430148	3.203899482070654
O	0.112106612189664	0.139406439096570	2.158163260758064
O	-0.756824548482506	-0.813952773410151	2.844815154780918

Transition Metal: Cr; Functional Group: H; Adsorbate: Clean

Cr	0.000000000000000	-0.000419450774408	0.004263861611150
C	0.686258318304940	4.264944496162618	-0.008630458198677
C	1.111225108148728	2.880442176457790	-0.005069024851562
C	2.442133197371728	2.441989580932540	-0.001037933605156
C	-0.686188200936453	-4.264982968514303	-0.005673838090985
C	-1.111213049258939	-2.880671533741580	0.000316999410258
C	-2.442226758736091	-2.442182452580390	0.001104675986510
C	0.686188200936466	-4.264982968514303	-0.005673838090985
C	1.111213049258938	-2.880671533741580	0.000316999410258
C	-0.686258318304944	4.264944496162618	-0.008630458198677
C	2.442226758736096	-2.442182452580390	0.001104675986510
C	-4.265378469941606	0.686497532270148	0.005073074253538
C	-1.111225108148734	2.880442176457790	-0.005069024851562
C	-2.880953562797785	1.111261444948100	0.005277550058048
C	-4.265600472550711	-0.685973076669637	0.004221437812494
C	-2.881144468402120	-1.111311763192468	0.005174681277102
C	-2.442133197371728	2.441989580932540	-0.001037933605156
C	4.265378469941608	0.686497532270148	0.005073074253538
C	2.880953562797784	1.111261444948100	0.005277550058048
C	4.265600472550714	-0.685973076669637	0.004221437812494
C	2.881144468402124	-1.111311763192468	0.005174681277102
N	0.000000000000000	2.048573446377900	-0.003270697876078
N	0.000000000000000	-2.048803121113007	0.004085918374438
N	-2.049219478213015	-0.000119034670338	0.007012361188244
N	2.049219478213018	-0.000119034670338	0.007012361188244
H	5.122363168345104	-1.357354475877500	0.000622303555502
H	-5.121821618183498	1.358350128808392	0.002029699014208
H	-5.122363168345100	-1.357354475877500	0.000622303555502
H	-1.358019637405082	5.121487743504316	-0.009565344732440
H	1.358019637405086	5.121487743504316	-0.009565344732440
H	5.121821618183500	1.358350128808392	0.002029699014208
H	-1.357866531097756	-5.121410855717443	-0.010219974312342
H	1.357866531097748	-5.121410855717443	-0.010219974312342
H	-3.214376760400476	3.214349553808892	-0.002383799630702
H	3.214376760400474	3.214349553808892	-0.002383799630702
H	-3.214523805769652	-3.214781933174262	-0.003946950189054
H	3.214523805769652	-3.214781933174262	-0.003946950189054

Transition Metal: Cr; Functional Group: H; Adsorbate: O

Cr	0.000000000000000	-0.000322412140704	0.517886593167952
C	0.685446528215480	4.231982076870348	-0.040040690775530
C	1.105047215987836	2.849491330969708	0.005691598097892
C	2.436524023677740	2.430787680353356	0.012829159457134
C	-0.685405329935687	-4.233843188411727	-0.039554117356321
C	-1.104936515308736	-2.851400650493009	0.007790971624056
C	-2.436404633540032	-2.4327444493827670	0.013387202703900
C	0.685405329935688	-4.233843188411727	-0.039554117356321
C	1.104936515308734	-2.851400650493009	0.007790971624056
C	-0.685446528215479	4.231982076870348	-0.040040690775530
C	2.436404633540038	-2.4327444493827670	0.013387202703900
C	-4.248127538088291	0.684209277603836	-0.021900838033233
C	-1.105047215987835	2.849491330969708	0.005691598097892
C	-2.863864034365932	1.102816966794566	0.023780978806416
C	-4.247917482432674	-0.686308357575463	-0.022668126816185
C	-2.863647774268298	-1.104729748818457	0.023374887708960
C	-2.436524023677734	2.430787680353356	0.012829159457134
C	4.248127538088282	0.684209277603836	-0.021900838033233
C	2.863864034365924	1.102816966794566	0.023780978806416
C	4.247917482432678	-0.686308357575463	-0.022668126816185
C	2.863647774268290	-1.104729748818457	0.023374887708960
N	0.000000000000000	2.008317791225842	0.030656620846892
N	0.000000000000000	-2.010064681394081	0.033952356924806
N	-2.024134235411051	-0.000881068249732	0.054799039757594
N	2.024134235411054	-0.000881068249732	0.054799039757594
H	5.100092278190528	-1.362663499919631	-0.059142359175084
H	-5.100684998681345	1.359974619097768	-0.056814217533663
H	-5.100092278190530	-1.362663499919631	-0.059142359175084
H	-1.361901557012764	5.084297480084988	-0.071307494633878
H	1.361901557012762	5.084297480084988	-0.071307494633878
H	5.100684998681349	1.359974619097768	-0.056814217533663
H	-1.361777905277300	-5.086107338054454	-0.073277108564870
H	1.361777905277308	-5.086107338054454	-0.073277108564870
H	-3.205137058792587	3.206030675433044	-0.009923068766734
H	3.205137058792594	3.206030675433044	-0.009923068766734
H	-3.205093909671699	-3.207957307787712	-0.010211030695442
H	3.205093909671700	-3.207957307787712	-0.010211030695442
O	0.000000000000000	0.002540394169604	2.112744857449812

Transition Metal: Cr; Functional Group: H; Adsorbate: OH

Cr	0.000000000000000	-0.000362544504566	0.307291466263196
C	0.686452807326246	4.256299498428650	-0.025321155604960
C	1.110715469202172	2.874302522113232	0.018867291509508
C	2.441309767844992	2.438371264658568	0.012569178233050
C	-0.685997914111031	-4.257687656215865	-0.022806322775910
C	-1.109010835639033	-2.873879401381902	0.013963938882372
C	-2.439193468881310	-2.438609807515078	0.012901131515204
C	0.685997914111032	-4.257687656215865	-0.022806322775910
C	1.109010835639038	-2.873879401381902	0.013963938882372
C	-0.686452807326255	4.256299498428650	-0.025321155604960
C	2.439193468881304	-2.438609807515078	0.012901131515204
C	-4.260083293777308	0.684651012031308	-0.026749297741450
C	-1.110715469202173	2.874302522113232	0.018867291509508
C	-2.874931555319137	1.108710010604164	0.006265779868048
C	-4.258750014579714	-0.686100716291051	-0.025523849392734
C	-2.873118783128994	-1.108699583015355	0.007944728154614
C	-2.441309767844999	2.438371264658568	0.012569178233050
C	4.260083293777305	0.684651012031308	-0.026749297741450
C	2.874931555319130	1.108710010604164	0.006265779868048
C	4.258750014579724	-0.686100716291051	-0.025523849392734
C	2.873118783128996	-1.108699583015355	0.007944728154614
N	0.000000000000000	2.040879007798122	0.046235420495928
N	0.000000000000000	-2.041779261129406	0.033906101999206
N	-2.041509539285535	0.000222138732964	0.021782187018022
N	2.041509539285538	0.000222138732964	0.021782187018022
H	5.112517327223158	-1.360761341236742	-0.049487461128933
H	-5.114873668066547	1.357970900422566	-0.051352812288293
H	-5.112517327223166	-1.360761341236742	-0.049487461128933
H	-1.359345498985078	5.111162816858922	-0.061444965816946
H	1.359345498985072	5.111162816858922	-0.061444965816946
H	5.114873668066540	1.357970900422566	-0.051352812288293
H	-1.359348284475768	-5.112422709793638	-0.050820290746113
H	1.359348284475756	-5.112422709793638	-0.050820290746113
H	-3.213423481326988	3.210494413719720	-0.006051987730772
H	3.213423481326990	3.210494413719720	-0.006051987730772
H	-3.211675090967894	-3.210408369302836	-0.000318390119310
H	3.211675090967892	-3.210408369302836	-0.000318390119310
H	0.000000000000000	0.899895268189116	2.519849067193206
O	0.000000000000000	-0.008742455988276	2.163512540377058

Transition Metal: Cr; Functional Group: H; Adsorbate: OOH

Cr	-0.003047340038738	-0.000954525723504	0.328443913536114
C	0.678854533958882	4.261178211720366	-0.026793618454803
C	1.100774232950206	2.876346052491716	0.020598981516826
C	2.430460785861896	2.441347888053102	0.020202877928070
C	-0.694959068788496	-4.257050682895049	-0.024024478850052
C	-1.118770763203120	-2.872387388663814	0.020734782401432
C	-2.447606233098156	-2.436397698395265	0.013734610396242
C	0.675945292761098	-4.256826311189100	-0.018305385145496
C	1.099210610635320	-2.872156483501577	0.028801276482754
C	-0.692386726104488	4.263330920662334	-0.031470415807853
C	2.428836698927336	-2.438167091187875	0.028185555435250
C	-4.264488745773090	0.689362791154860	-0.040591881423261
C	-1.117649235352431	2.879195973746556	0.013616875437672
C	-2.881621513533027	1.113068513470422	0.004723190135556
C	-4.263357834783774	-0.682975058915709	-0.039315585596142
C	-2.880522504971342	-1.105298677684747	0.007823194671660
C	-2.447954656436913	2.444557015062690	0.008843714824958
C	4.249577951638682	0.686893879385922	-0.018364688578806
C	2.866130467526822	1.110753528118882	0.013541987315904
C	4.249004561451367	-0.685417027035133	-0.0154431111107551
C	2.865194968859022	-1.107780508776383	0.018349295723162
N	-0.009677883337920	2.045450307824916	0.044728781613902
N	-0.010305275319114	-2.040636422912506	0.051705950931900
N	-2.048371283324911	0.004079256625568	0.032416399581820
N	2.034608658317892	0.001899947992950	0.027071252253396
H	5.103699391294048	-1.359145008074318	-0.037820601988216
H	-5.119286092829405	1.362001103559982	-0.077716391650064
H	-5.117322072947896	-1.356894458747142	-0.073762430516005
H	-1.364454729294302	5.118662737985584	-0.072620932139081
H	1.353785492010994	5.114461412214956	-0.061839533603237
H	5.104898133318629	1.359667296705914	-0.043249366075308
H	-1.368114827382051	-5.111501896423301	-0.062762702517109
H	1.350031321307572	-5.110711323847308	-0.051203955142419
H	-3.220703275499027	3.216159163238684	-0.015458540247450
H	3.202819439381250	3.213561770800054	0.006321037092108
H	-3.220884539358483	-3.207359031852121	-0.008198659899880
H	3.200718565017276	-3.210799021732512	0.016246214731882
H	-1.240178950474263	0.623426462207324	3.185044942459680
O	0.275564874463370	0.031724622089222	2.186073405925338
O	-0.935452427830629	-0.279250237554475	2.948424038346576

Transition Metal: Cr; Functional Group: NH2; Adsorbate: Clean

Cr	0.038703894490450	-0.017085711120310	-0.057675174410788
C	0.883745696264564	4.213795300898628	-0.383577896510802
C	1.253158304235300	2.816593234042594	-0.365451231003206
C	2.576075918648402	2.305997417770592	-0.459324676226604
C	-0.791526688488954	-4.251081819226366	-0.213358871469312
C	-1.175428368296828	-2.858864608764932	-0.175725494060432
C	-2.489157653067590	-2.358633916819983	-0.308152272064584
C	0.586994640752916	-4.299421398502922	-0.079546740569220
C	1.038005627657298	-2.934374816948374	0.115043245992908
C	-0.481868882158963	4.279844357654440	-0.144825064672022
C	2.377817142595584	-2.546001338769734	0.371121987633980
C	-4.193636259461437	0.810783037043648	0.280353080171952
C	-0.963889125777225	2.916016020214892	-0.056938018674330
C	-2.809886796069993	1.209024040723232	0.149147967402148
C	-4.238055872536528	-0.571663487647950	0.156042130894486
C	-2.880422356061096	-1.016896568080501	-0.054202055219402
C	-2.326952440611649	2.543322027680344	0.057630404694054
C	4.306554752437666	0.551916659096790	0.155295786443274
C	2.955602391101796	0.972917289258894	-0.167474761500098
C	4.243924474008132	-0.800077395603441	0.464945665245950
C	2.868108697315610	-1.217226058258412	0.296874528591322
N	0.119358638034594	2.040063144686358	-0.149462372505166
N	-0.046858723682696	-2.067226679604545	0.041460234683664
N	-2.017144500228888	0.074317792094646	0.004170475607268
N	2.093268081969284	-0.113308086409916	-0.054037829395966
N	5.364250559893494	-1.628462025649281	0.841021693534038
N	-5.325630364585315	1.675084288756622	0.469911234599746
N	-5.410989131386007	-1.354656520199843	0.223090888156930
N	-1.222208114958075	5.471700815020264	-0.039189362301416
N	1.763955129131278	5.339252812300634	-0.576400376770294
N	5.471300641660468	1.330039959146584	0.169494700810952
N	-1.637637420818191	-5.387987180252711	-0.378785861610996
N	1.349601167296548	-5.491971764517720	-0.110723388345222
N	-3.284073751966979	3.595810039051824	0.059197779980108
N	3.631974490775096	3.213901534723234	-0.766932465975906
N	-3.523993724976183	-3.272900722032340	-0.671171244025478
N	3.301781693099002	-3.599777579063460	0.640389346992752
H	-2.452582022223918	-5.342499900791683	0.240344432432196
H	-1.127542375015242	-6.242421223217477	-0.138369876231066
H	-3.157868650507424	-4.080722339919570	-1.179590148535617
H	-4.240165566960846	-2.822112425137874	-1.242862409643990
H	-5.519421641291864	1.876029968107950	1.456564024371534
H	-6.173097322666049	1.287860185275768	0.048674443691944
H	-2.029266779938315	5.384825972030382	0.581779895978556
H	1.331452018217964	6.054905704900015	-1.166842164891126
H	2.038810946754886	5.785013440567178	0.306116275186798
H	3.269534444517024	4.154360706690856	-0.969556371389958
H	4.210244256237152	2.877246243517054	-1.539311761437922
H	5.273540960642146	2.332049101908926	0.238954072580108
H	6.154265646882681	1.018041761552424	0.861331862214708
H	6.181224808809800	-1.431710979319611	0.254312553750876
H	5.645704739818964	-1.479156672798009	1.816448867025444
H	4.254256644103868	-3.232516699063108	0.763431439292428
H	3.030161727872624	-4.150093018768166	1.458609186189632
H	2.347751247144134	-5.277835499309360	-0.200349501020305
H	1.064383899591014	-6.105736152960473	-0.877806276637676
H	-5.234377224985955	-2.312300650541069	0.532244807711404
H	-6.125571546717390	-0.924669764513666	0.814299683007940
H	-4.243236543071793	3.229578100610964	0.017803393055162
H	-3.125283535911013	4.262879832880526	-0.698551913628094
H	-0.637481756657358	6.265317732586400	0.230234276862594

Transition Metal: Cr; Functional Group: NH2; Adsorbate: O

Cr	0.025712443120614	-0.006045990565904	0.490731579943124
C	0.883493700566128	4.137727206650056	-0.472723610711139
C	1.233227227925544	2.739821376906730	-0.427863433066268
C	2.548140849310974	2.225559986554106	-0.560446320220969
C	-0.776161700850796	-4.184304466041038	-0.376101866618963
C	-1.160657546163442	-2.796570604132064	-0.291052699269237
C	-2.466135703007442	-2.301918455946641	-0.461430062310313
C	0.584592164851598	-4.245359145081595	-0.120829502305313
C	1.011836718811236	-2.896340573905341	0.176374624556202
C	-0.455167837782863	4.231602288089816	-0.120298949381137
C	2.326576981199014	-2.533633427838286	0.548357314390330
C	-4.168325162664402	0.804978945351352	0.359159659304608
C	-0.944101947343267	2.880423943116640	0.036234499149438
C	-2.784929579875545	1.203992926752468	0.259662338267456
C	-4.215211610794825	-0.562950583239555	0.125563141424150
C	-2.858247633343190	-0.988419597143164	-0.107200279699143
C	-2.305002660380289	2.536796725617924	0.217611107676054
C	4.265918593353287	0.520163857434466	0.176967110395928
C	2.916426649719116	0.921953029401732	-0.171384740130922
C	4.190078171253800	-0.799468384435293	0.600612922484042
C	2.815097935071672	-1.213289341725886	0.449931665375556
N	0.114162531045502	1.979199046597328	-0.103082764582080
N	-0.054740218257898	-2.011731585370999	0.051111433688390
N	-1.985688842707766	0.084853029025484	0.044870435296214
N	2.037538056658548	-0.137045406630378	0.029315273179362
N	5.290781161890362	-1.613630140346160	1.052444076002706
N	-5.293126794060157	1.660211235114160	0.610583848620816
N	-5.385551331312854	-1.353629780282578	0.123244203873142
N	-1.171751334338776	5.437748325374344	0.015362009557416
N	1.763411108362950	5.237962850091035	-0.775016307546576
N	5.435116569662636	1.288638355494464	0.120639589546498
N	-1.594199397911527	-5.309289691794612	-0.676313891569272
N	1.348249729530056	-5.435643699309107	-0.149739425425640
N	-3.245595408925091	3.589386208450498	0.299154058066514
N	3.590525624126910	3.095684333777172	-0.979265915516777
N	-3.474642722229973	-3.182716669552185	-0.946726301059140
N	3.215505270952100	-3.586787698918460	0.898234104952460
H	-2.487839065034457	-5.274255132538407	-0.178409741524812
H	-1.119638443345732	-6.171635360867304	-0.394766591083531
H	-3.090632079344076	-3.914053329371228	-1.547795310432750
H	-4.207162584454968	-2.682941443735402	-1.452722300303495
H	-5.471286880440136	1.806618831213832	1.609528566383806
H	-6.148713054761535	1.305749525371052	0.177774902861826
H	-1.860241364545029	5.406631429652061	0.770259893114860
H	1.297254059533334	5.948913233698148	-1.344199536649210
H	2.129459071154932	5.696653428512331	0.066587704473516
H	3.229434929795236	4.019056872191434	-1.247955784584626
H	4.161674787950016	2.688018845419724	-1.721137819077860
H	5.247249675735546	2.294509377202916	0.105795932731248
H	6.118196416003076	1.031179534548412	0.834348513487756
H	6.121146531984274	-1.472864294460425	0.468741387249376
H	5.555018892388030	-1.399955303481320	2.020507742307166
H	4.161726228939984	-3.229913900979547	1.080277296994412
H	2.875727626314562	-4.136755251718906	1.689768455678990
H	2.349988398849346	-5.223750411909094	-0.102948492215177
H	1.153626402327238	-5.991034255329286	-0.986625420114969
H	-5.211152662517609	-2.324876226983978	0.387642975790848
H	-6.110749394901339	-0.960680010047575	0.726894270666944
H	-4.210695605040261	3.242363028586558	0.245799809738806
H	-3.078758021054536	4.325202720903624	-0.389250781199653
H	-0.545704796885410	6.235332668646754	0.145866309205472
O	0.025175016767830	0.066192909084600	2.092218731673142

Transition Metal: Cr; Functional Group: NH2; Adsorbate: OH

Cr	0.021603066622718	-0.012555336394694	0.294071909970422
C	0.883486870001044	4.172564797770740	-0.422069139802147
C	1.243535906439576	2.774205049104374	-0.375613259590331
C	2.561072969627222	2.251360990729644	-0.494538066617423
C	-0.804594012421894	-4.218883766066881	-0.321493598210008
C	-1.186014117804149	-2.826250528570434	-0.268141075162173
C	-2.485310223370185	-2.314464283586496	-0.467440860925279
C	0.554710340275678	-4.281621627731965	-0.058434618474806
C	0.991868775170266	-2.924639447664529	0.207070160982394
C	-0.460632270490176	4.259111934184120	-0.084513899041930
C	2.316644507442598	-2.545378948934875	0.541553115171710
C	-4.195765164945154	0.815745129753850	0.293127636989670
C	-0.948629240450082	2.906037578509170	0.072331731777368
C	-2.806265650879162	1.210817247272762	0.230548008474140
C	-4.245235508887284	-0.549279820739915	0.041083435842858
C	-2.883575878048248	-0.985302571862189	-0.160764010912981
C	-2.313096219205455	2.544715023888550	0.236956948328558
C	4.283496909217140	0.507560401006156	0.171352674602508
C	2.933632375033724	0.929163965072666	-0.157566635977425
C	4.204501675671867	-0.823268019371177	0.560993302168456
C	2.823845649416580	-1.228878548921255	0.420127445021808
N	0.118356620585360	2.018063888864314	-0.067206347913707
N	-0.076183309727135	-2.050073497358635	0.065342113594024
N	-2.018960139129174	0.088155499314208	0.006551847826224
N	2.060314161335748	-0.139199958747760	0.012989759547542
N	5.310535990981430	-1.651413576490842	0.976584213326764
N	-5.324201352284064	1.672276518638502	0.529737408533056
N	-5.422027893528297	-1.328038679613908	-0.004661547774144
N	-1.192760327090053	5.461910608946228	0.018502370853822
N	1.762103356156346	5.279110179736626	-0.713538057743509
N	5.458139585874497	1.267599441344064	0.118940262254636
N	-1.635629910256423	-5.339856578945168	-0.616824469098951
N	1.316364760533746	-5.474227972015875	-0.060730063979207
N	-3.253452325152253	3.591120680371190	0.358989505168586
N	3.612716452154734	3.136522056324394	-0.861015173199561
N	-3.495692486380797	-3.1996026245250600	-0.938962677749618
N	3.207973609388540	-3.597249671062482	0.895020021412494
H	-2.494212650661680	-5.327929840087384	-0.057820016898446
H	-1.144596688822645	-6.208759646947598	-0.389605564061178
H	-3.107321314205915	-3.987353360322722	-1.461302014575313
H	-4.188054539056989	-2.718525658928719	-1.514449084120059
H	-5.535337659156641	1.788036040537340	1.526428353506470
H	-6.166728909350239	1.336005247777308	0.057952980732466
H	-1.822498943015006	5.475488989387842	0.823962698962012
H	1.353160024199642	5.920156830709928	-1.399007784708566
H	2.002422939768142	5.823232471846346	0.122320826022508
H	3.255656682089738	4.074876176204298	-1.081188737144437
H	4.180082040706806	2.767291402507562	-1.626128754895650
H	5.279934843363142	2.274626169029438	0.153941620029714
H	6.159544069040912	0.970603318046274	0.798469578777372
H	6.118104311133514	-1.533406434232141	0.356549603870040
H	5.619434957006230	-1.429547564473598	1.929427426559528
H	4.160668666795508	-3.242610700117957	1.047404980011620
H	2.883086072182904	-4.121264885028639	1.710274481999864
H	2.318291368440130	-5.259941823133907	-0.025859013108512
H	1.120553840674930	-6.051159027665163	-0.882747420071667
H	-5.262514122963546	-2.303533162613537	0.254531738509910
H	-6.162228707557066	-0.933415149545784	0.579681145917244
H	-4.218851326345481	3.251921695540752	0.267267444394612
H	-3.068490596220602	4.371529492166638	-0.273333814297271
H	-0.573327523634447	6.274713014962511	0.052751915009250
H	0.494923813366604	0.892814862449234	2.457857103763960
O	0.021679941223420	0.090547959610684	2.167766327770656

Transition Metal: Cr; Functional Group: NH2; Adsorbate: OOH

Cr	0.026949969205344	-0.018345178268998	0.308677501090414
C	0.884895831430952	4.171034505035274	-0.428925485982965
C	1.241216326221920	2.770862593865884	-0.380392404510783
C	2.557710478786984	2.246589970895254	-0.501933650962030
C	-0.807906083180875	-4.219245781544988	-0.321870944519468
C	-1.186905266659355	-2.825812772124056	-0.264773968579995
C	-2.482845526432641	-2.309777886927812	-0.469500069101695
C	0.550379988027936	-4.284892592336913	-0.056748626642900
C	0.988943481435444	-2.928457615619948	0.213588392011918
C	-0.456394693766267	4.261463432439180	-0.084784938586754
C	2.314472898956134	-2.550013639210672	0.543383643100104
C	-4.191169465728770	0.818560275806012	0.303039402152232
C	-0.946226672595095	2.908568185364130	0.075275018336724
C	-2.803288911472986	1.215951132831312	0.240863626828864
C	-4.239238619689473	-0.546779360427042	0.045245754009382
C	-2.878747457409631	-0.981069994908342	-0.157522142438879
C	-2.310065909370479	2.550568433491632	0.249219464846790
C	4.279197573229368	0.505648806200182	0.170577811537238
C	2.931221782459658	0.923450785631966	-0.167542734554250
C	4.200664136147142	-0.826596777605477	0.558365928217424
C	2.823115646676260	-1.234197501187754	0.411043088078104
N	0.116778134016022	2.018413148424144	-0.068012946268581
N	-0.077894008845291	-2.052828193827796	0.075368249379532
N	-2.013460903096021	0.093047087902434	0.014246752024014
N	2.060376367774080	-0.147383842628301	-0.004832836333852
N	5.302979554751440	-1.651940278039479	0.987629940413016
N	-5.324440793709170	1.672084462323470	0.531083269211280
N	-5.416368561245918	-1.322597065381288	-0.006130068750132
N	-1.187227447195486	5.465348221101132	0.020455123226706
N	1.763949973524480	5.274952986522400	-0.729186555960453
N	5.451520978007470	1.269666910125892	0.133388401462080
N	-1.642577096746546	-5.336359135257460	-0.622096119848411
N	1.311210666140416	-5.477923072750317	-0.063548357002865
N	-3.250397632800329	3.596460755907830	0.381454576014020
N	3.609158246630654	3.131099663053532	-0.866022379978489
N	-3.494086955810836	-3.187434835158712	-0.955002413860203
N	3.203111406875554	-3.599929760926933	0.904952032323072
H	-2.498715697978618	-5.326357223144436	-0.059408560071898
H	-1.152483651566506	-6.207188274537419	-0.400844183422869
H	-3.102713137147106	-3.980815364591706	-1.466993915536165
H	-4.167725898230279	-2.701254571789477	-1.548563731642382
H	-5.562186833625798	1.766738512645322	1.524115191865250
H	-6.154246043114910	1.342585182141494	0.031928872325632
H	-1.806203761191515	5.483621834451368	0.834166564799816
H	1.349099624629150	5.918357711029922	-1.408764966988937
H	2.015758261660822	5.816181801462562	0.105153811970180
H	3.254387644069498	4.069504892063252	-1.089670111837727
H	4.184965579519576	2.760847211222946	-1.624166351987164
H	5.267971438777880	2.276004077583096	0.167290318778174
H	6.143155284323733	0.975898832847174	0.824513072267646
H	6.116081706556490	-1.535990092870325	0.374599622234266
H	5.603198894007861	-1.424555938035517	1.942092411454340
H	4.155668428581888	-3.245516441427721	1.059763022039072
H	2.873310366144150	-4.120989760445394	1.720083828795114
H	2.313075142161066	-5.265510925492142	-0.019196453665412
H	1.121740167124596	-6.046282792732882	-0.892928822763022
H	-5.255863655809392	-2.306310106482659	0.219398536311436
H	-6.151779948793287	-0.943429729760680	0.594005587066752
H	-4.215419178978312	3.256627121416614	0.290336952424744
H	-3.068756926570025	4.379368209343922	-0.248662559868823
H	-0.566319541140953	6.277401060326771	0.044481280491490
H	-1.290539971089807	0.579081307902448	3.128821360305238
O	0.294764449624560	0.092284763567744	2.177338080084254
O	-0.885246294038396	-0.299701015620574	2.969505161018084

Transition Metal: Cr; Functional Group: OH; Adsorbate: Clean

Cr	10.996029999999999	11.014040000000000	7.851800000000000
C	10.329029999999999	15.270440000000001	7.759270000000000
C	9.908939999999999	13.899459999999999	7.756230000000000
C	8.572530000000000	13.458170000000001	7.702000000000000
C	11.660980000000000	6.758600000000000	7.738040000000000
C	12.083080000000001	8.128399999999999	7.777640000000000
C	13.421400000000000	8.566970000000000	7.792010000000000
C	10.283950000000001	6.728660000000000	7.837990000000000
C	9.849090000000000	8.106550000000000	7.889970000000000
C	11.708399999999999	15.298410000000001	7.817030000000000
C	8.509650000000001	8.555099999999999	7.947850000000000
C	15.257410000000000	11.671090000000000	7.997520000000000
C	12.142080000000000	13.920760000000000	7.876950000000000
C	13.890900000000000	12.122059999999999	7.951000000000000
C	15.252520000000001	10.295410000000000	7.933570000000000
C	13.868650000000001	9.895630000000001	7.857600000000000
C	13.480710000000000	13.473070000000000	7.959010000000000
C	6.738090000000000	11.729240000000001	7.799120000000000
C	8.123670000000001	12.129820000000000	7.770560000000000
C	6.732160000000000	10.355869999999999	7.904760000000000
C	8.099800000000000	9.906129999999999	7.916930000000000
N	11.027900000000001	13.079560000000001	7.832230000000000
N	10.963889999999999	8.947760000000001	7.854490000000000
N	13.044540000000000	11.016900000000000	7.870400000000000
N	8.947369999999999	11.010800000000000	7.844260000000000
O	9.483040000000001	16.394220000000001	7.655650000000000
O	7.556240000000000	14.408510000000000	7.587910000000000
O	12.506320000000001	5.629200000000000	7.693970000000000
O	14.440120000000000	7.612180000000000	7.760410000000000
O	9.487450000000001	5.615550000000000	7.868000000000000
O	12.509160000000000	16.409710000000000	7.819440000000000
O	7.561930000000000	7.561040000000000	8.013710000000000
O	16.354700000000001	12.511889999999999	8.088070000000000
O	16.387380000000000	9.524770000000000	7.950010000000000
O	14.426570000000000	14.467639999999999	8.043480000000001
O	5.602850000000000	12.498089999999999	7.748060000000000
O	5.633380000000000	9.515480000000000	7.982160000000000
H	9.460910000000000	16.851310000000002	8.519150000000000
H	7.969360000000000	15.299670000000001	7.525640000000000
H	12.491580000000001	5.263440000000000	6.787830000000000
H	14.029949999999999	6.718740000000000	7.808350000000000
H	10.075820000000000	4.841890000000000	7.971790000000000
H	11.950160000000000	17.171800000000001	7.570690000000000
H	6.669150000000000	7.964890000000000	8.017760000000001
H	17.165710000000001	11.970050000000001	8.090830000000000
H	16.094120000000000	8.589850000000000	7.901250000000000
H	15.318910000000001	14.063990000000000	8.075329999999999
H	5.896580000000000	13.430050000000000	7.661330000000000
H	4.821840000000000	10.052080000000000	7.912790000000000

Transition Metal: Cr; Functional Group: OH; Adsorbate: O

Cr	10.994330000000000	11.014720000000001	7.694430000000000
C	10.328960000000000	15.230350000000000	6.961640000000000
C	9.919219999999999	13.858510000000001	6.991580000000000
C	8.593760000000000	13.416309999999999	6.866860000000000
C	11.657190000000000	6.799770000000000	6.928370000000000
C	12.073689999999999	8.169200000000000	6.994060000000000
C	13.406160000000000	8.603350000000001	6.935620000000000
C	10.301679999999999	6.755190000000000	7.181050000000000
C	9.877359999999999	8.128060000000000	7.328440000000000
C	11.695340000000000	15.271170000000000	7.149110000000000
C	8.545590000000001	8.560650000000001	7.476860000000000
C	15.216830000000000	11.681570000000001	7.375040000000000
C	12.118850000000000	13.899430000000001	7.303660000000000
C	13.849869999999999	12.122420000000000	7.380880000000000
C	15.218579999999999	10.320860000000000	7.167080000000000
C	13.836220000000001	9.925640000000000	7.081800000000000
C	13.448440000000000	13.467570000000000	7.473300000000000
C	6.779530000000000	11.694500000000000	7.044770000000000
C	8.162850000000001	12.093750000000000	7.009510000000000
C	6.776700000000000	10.339680000000000	7.289870000000000
C	8.143660000000001	9.903910000000000	7.356520000000000
N	11.022760000000000	13.041560000000000	7.200780000000000
N	10.973080000000000	8.986260000000000	7.217800000000000
N	12.996160000000000	11.030820000000000	7.207730000000000
N	8.999870000000000	10.994470000000000	7.191640000000000
O	10.984330000000000	11.022040000000001	9.292380000000000
O	9.487690000000001	16.335270000000001	6.718140000000000
O	7.585670000000000	14.344640000000000	6.622530000000000
O	12.496940000000000	5.683260000000000	6.730530000000000
O	14.421889999999999	7.664240000000000	6.768990000000000
O	9.507870000000000	5.642940000000000	7.243400000000000
O	12.497130000000000	16.381480000000000	7.162940000000000
O	7.613560000000000	7.574930000000000	7.675310000000000
O	16.307860000000002	12.518520000000001	7.528950000000000
O	16.356670000000001	9.561950000000000	7.079720000000000
O	14.376410000000000	14.454459999999999	7.684590000000000
O	5.643200000000000	12.446610000000000	6.895460000000000
O	5.683170000000000	9.502500000000000	7.427780000000000
H	9.416890000000000	16.861170000000001	7.538730000000000
H	7.995510000000000	15.237349999999999	6.550660000000000
H	12.401300000000001	5.380180000000000	5.806310000000000
H	14.020040000000000	6.765340000000000	6.792150000000000
H	10.098580000000000	4.864450000000000	7.222810000000000
H	11.974010000000000	17.124580000000002	6.803500000000000
H	6.717040000000000	7.971200000000000	7.675660000000000
H	17.123729999999998	11.988160000000001	7.462810000000000
H	16.069320000000001	8.632560000000000	6.951140000000000
H	15.272259999999999	14.057580000000000	7.709520000000000
H	5.931480000000000	13.370670000000000	6.736490000000000
H	4.869000000000000	10.024500000000000	7.301060000000000

Transition Metal: Cr; Functional Group: OH; Adsorbate: OH

Cr	10.991370000000000	11.010970000000000	7.376960000000000
C	10.322229999999999	15.248650000000000	6.919980000000000
C	9.907159999999999	13.876749999999999	6.923430000000000
C	8.575089999999999	13.433009999999999	6.826440000000000
C	11.655989999999999	6.774160000000000	6.866660000000000
C	12.079480000000000	8.142049999999999	6.932770000000000
C	13.416660000000000	8.579359999999999	6.904790000000000
C	10.287900000000000	6.737280000000000	7.052560000000000
C	9.857699999999999	8.111070000000000	7.174240000000000
C	11.695530000000000	15.282500000000001	7.058390000000000
C	8.520540000000000	8.554860000000000	7.281320000000000
C	15.243460000000001	11.673909999999999	7.231630000000000
C	12.125109999999999	13.906950000000000	7.164820000000000
C	13.874169999999999	12.117490000000000	7.226230000000000
C	15.244870000000001	10.305890000000000	7.078430000000000
C	13.860790000000000	9.905250000000001	7.004130000000000
C	13.459960000000001	13.463930000000000	7.298800000000000
C	6.744160000000000	11.705380000000000	6.944930000000000
C	8.130300000000000	12.106629999999999	6.920260000000000
C	6.739870000000000	10.341570000000001	7.131370000000000
C	8.108720000000000	9.900150000000000	7.184300000000000
N	11.020390000000001	13.062020000000000	7.070550000000000
N	10.966460000000000	8.957440000000000	7.099540000000000
N	13.031370000000001	11.018300000000000	7.083640000000000
N	8.955719999999999	10.997080000000000	7.052860000000000
O	10.978690000000000	11.048010000000000	9.242640000000000
O	9.478529999999999	16.363610000000001	6.739540000000000
O	7.564880000000000	14.375170000000001	6.647420000000000
O	12.496040000000001	5.650600000000000	6.716950000000000
O	14.432000000000000	7.629540000000000	6.799220000000000
O	9.490500000000001	5.625600000000000	7.079880000000000
O	12.497080000000000	16.392749999999999	7.074190000000000
O	7.583350000000000	7.564230000000000	7.435870000000000
O	16.335000000000001	12.518260000000000	7.345190000000000
O	16.383099999999999	9.543080000000000	7.013640000000000
O	14.393420000000001	14.454710000000000	7.469470000000000
O	5.609350000000000	12.464740000000001	6.819000000000000
O	5.646020000000000	9.497669999999999	7.225850000000000
H	11.232570000000001	10.182160000000000	9.614179999999999
H	9.422790000000001	16.852860000000000	7.583730000000000
H	7.978180000000000	15.266920000000001	6.585270000000000
H	12.436680000000001	5.335240000000000	5.793740000000000
H	14.024080000000000	6.733900000000000	6.821350000000000
H	10.080740000000000	4.846770000000000	7.097730000000000
H	11.958159999999999	17.146360000000001	6.763340000000000
H	6.687380000000000	7.961690000000000	7.425400000000000
H	17.150710000000000	11.984760000000000	7.310400000000000
H	16.095210000000002	8.609620000000000	6.927760000000000
H	15.289000000000000	14.056929999999999	7.492030000000000
H	5.900240000000000	13.394520000000000	6.706060000000000
H	4.831830000000000	10.025210000000000	7.126260000000000

Transition Metal: Cr; Functional Group: OH; Adsorbate: OOH

Cr	10.984140000000000	11.034230000000001	6.847700000000000
C	10.326490000000000	15.283289999999999	6.392320000000000
C	9.906940000000001	13.912950000000000	6.422170000000000
C	8.570380000000000	13.477440000000000	6.370100000000000
C	11.648450000000000	6.791720000000000	6.391810000000000
C	12.069440000000000	8.160690000000001	6.452500000000000
C	13.407920000000001	8.593340000000000	6.465560000000000
C	10.272760000000000	6.760500000000000	6.499360000000000
C	9.841519999999999	8.137639999999999	6.578880000000000
C	11.704940000000001	15.311260000000001	6.454700000000000
C	8.502670000000000	8.580900000000000	6.646580000000000
C	15.245200000000001	11.692720000000000	6.635990000000000
C	12.133889999999999	13.934369999999999	6.552130000000000
C	13.877940000000001	12.140660000000000	6.621090000000000
C	15.239730000000000	10.318099999999999	6.564940000000000
C	13.853990000000000	9.921090000000000	6.519180000000000
C	13.471340000000000	13.490850000000000	6.647930000000000
C	6.737130000000000	11.750629999999999	6.423440000000000
C	8.122310000000001	12.150690000000001	6.437080000000000
C	6.729030000000000	10.377929999999999	6.535500000000000
C	8.095300000000000	9.930690000000000	6.595760000000000
H	9.457470000000001	16.893490000000000	7.084810000000000
H	7.975510000000000	15.315560000000000	6.153510000000000
H	12.470179999999999	5.323950000000000	5.391870000000000
H	14.010630000000001	6.744540000000000	6.456790000000000
H	10.059710000000001	4.872000000000000	6.576160000000000
H	11.954060000000000	17.174070000000000	6.143720000000000
H	6.663120000000000	7.990820000000000	6.711410000000000
H	17.154480000000000	11.997880000000000	6.681250000000000
H	16.084430000000001	8.613709999999999	6.505250000000000
H	15.306920000000000	14.081390000000001	6.773270000000000
H	5.896500000000000	13.448490000000000	6.241540000000000
H	4.822040000000000	10.066979999999999	6.441730000000000
H	9.448330000000000	10.718650000000000	9.625400000000001
O	9.481009999999999	16.402030000000000	6.240480000000000
O	7.558490000000000	14.427890000000000	6.244660000000000
O	12.493880000000001	5.665560000000000	6.307370000000000
O	14.422409999999999	7.638750000000000	6.432230000000000
O	9.473260000000000	5.650500000000000	6.503620000000000
O	12.509779999999999	16.417829999999999	6.416830000000000
O	7.557050000000000	7.589160000000000	6.723020000000000
O	16.341290000000001	12.536350000000001	6.690020000000000
O	16.374990000000000	9.550039999999999	6.533950000000000
O	14.413270000000001	14.483309999999999	6.747740000000000
O	5.603470000000000	12.515480000000000	6.316720000000000
O	5.630730000000000	9.535019999999999	6.562590000000000
O	11.066760000000000	11.180339999999999	8.722110000000001
O	10.245089999999999	10.184139999999999	9.421010000000001
N	11.022830000000001	13.092380000000000	6.516560000000000
N	10.952930000000000	8.980259999999999	6.546340000000000
N	13.028940000000000	11.039840000000000	6.545760000000000
N	8.945440000000000	11.032909999999999	6.539310000000000

Transition Metal: Cu; Functional Group: BH2; Adsorbate: Clean

H	8.329639999999999	16.654370000000000	6.242960000000000
H	10.004810000000000	17.667739999999998	6.911220000000000
H	6.200960000000000	13.792190000000000	8.392609999999999
H	6.774460000000000	15.421740000000000	7.386570000000000
H	11.704150000000000	4.335090000000000	7.001080000000000
H	13.372420000000000	5.312450000000000	6.270630000000000
H	14.880220000000000	6.587400000000000	7.335200000000000
H	15.612850000000000	8.225490000000001	6.415230000000000
H	8.961990000000000	4.922550000000000	8.313390000000000
H	8.721900000000000	5.109080000000000	6.272840000000000
H	13.682600000000001	15.632989999999999	6.211610000000000
H	12.927519999999999	17.324510000000000	7.042610000000000
H	6.223890000000000	7.696740000000000	7.588740000000000
H	7.665690000000000	6.261120000000000	7.591180000000000
H	16.465730000000001	13.466710000000001	8.472730000000000
H	17.490430000000000	11.903750000000000	7.586700000000000
H	15.502290000000000	8.202520000000000	8.339180000000001
H	17.169020000000000	8.976279999999999	7.478670000000000
H	13.663230000000000	15.778530000000000	8.132999999999999
H	15.286170000000000	14.999499999999999	7.228520000000000
H	4.527030000000000	12.994300000000001	7.553690000000000
H	6.064790000000000	13.773070000000001	6.470440000000000
H	4.877460000000000	8.901800000000000	6.574340000000000
H	4.972920000000000	8.971500000000001	8.636240000000001
C	10.145830000000000	15.318780000000000	7.110870000000000
C	9.670370000000000	13.917170000000000	7.213780000000000
C	8.334619999999999	13.438090000000001	7.285710000000000
C	11.588030000000000	6.679740000000000	7.170110000000000
C	12.046900000000001	8.090220000000000	7.214360000000000
C	13.355620000000000	8.589869999999999	7.258840000000000
C	10.193360000000000	6.730970000000000	7.295620000000000
C	9.843510000000000	8.141950000000000	7.345750000000000
C	11.544029999999999	15.227290000000000	7.178880000000000
C	8.485180000000000	8.543990000000001	7.428330000000000
C	15.134069999999999	11.722360000000000	7.467680000000000
C	11.877980000000001	13.832020000000000	7.270400000000000
C	13.729360000000000	12.189170000000001	7.392950000000000
C	15.052849999999999	10.327980000000000	7.384360000000000
C	13.653090000000001	9.979889999999999	7.318120000000000
C	13.253600000000000	13.511540000000000	7.327990000000000
C	6.657750000000000	11.667840000000000	7.437690000000000
C	8.053400000000000	12.068659999999999	7.349370000000000
C	6.641120000000000	10.279260000000001	7.480080000000000
C	8.063480000000000	9.892080000000000	7.416700000000000
B	9.418559999999999	16.628019999999999	6.747030000000000
B	6.943970000000000	14.239860000000000	7.368890000000000
B	12.299410000000000	5.365990000000000	6.804920000000000
B	14.730820000000000	7.770600000000000	7.323680000000000
B	9.105940000000000	5.586760000000000	7.314020000000000
B	12.832240000000001	16.135190000000001	7.129240000000000
B	7.441110000000000	7.479950000000000	7.528100000000000
B	16.444870000000002	12.440580000000001	7.849930000000000
B	15.976810000000000	9.053330000000001	7.413580000000000
B	14.098319999999999	14.874570000000000	7.239960000000000
B	5.720110000000000	12.926470000000000	7.472450000000000
B	5.487850000000000	9.212870000000001	7.569880000000000
Cu	10.868620000000000	11.015879999999999	7.314600000000000
N	10.747710000000000	13.050789999999999	7.293570000000000
N	10.945000000000000	8.944800000000001	7.296070000000000
N	12.864649999999999	11.099270000000001	7.319030000000000
N	8.891230000000000	10.969720000000001	7.340730000000000

Transition Metal: Cu; Functional Group: BH2; Adsorbate: O

C	10.144180000000000	15.324870000000001	6.745290000000000
C	9.666119999999999	13.923670000000000	6.844590000000000
C	8.335010000000000	13.440939999999999	6.918410000000000
C	11.588749999999999	6.673400000000000	6.812400000000000
C	12.047140000000001	8.085410000000000	6.851740000000000
C	13.353710000000000	8.589580000000000	6.897630000000000
C	10.194780000000000	6.725360000000000	6.945460000000000
C	9.845030000000000	8.138400000000001	6.991690000000000
C	11.541420000000000	15.231619999999999	6.823000000000000
C	8.486490000000000	8.544810000000000	7.078200000000000
C	15.140820000000000	11.722670000000001	7.099040000000000
C	11.875700000000000	13.833959999999999	6.914840000000000
C	13.735590000000000	12.193130000000000	7.036600000000000
C	15.055380000000000	10.328550000000000	7.012880000000000
C	13.654080000000000	9.981460000000000	6.953960000000000
C	13.254120000000000	13.513010000000000	6.979280000000000
C	6.655860000000000	11.666779999999999	7.064550000000000
C	8.052809999999999	12.067539999999999	6.976450000000000
C	6.639440000000000	10.277369999999999	7.106350000000000
C	8.060630000000000	9.889239999999999	7.047430000000000
B	9.416350000000000	16.634380000000000	6.381340000000000
B	6.943740000000000	14.241569999999999	7.005910000000000
B	12.299700000000000	5.360600000000000	6.442830000000000
B	14.730140000000000	7.769640000000000	6.961060000000000
B	9.104730000000000	5.584810000000000	6.957470000000000
B	12.829590000000000	16.138290000000001	6.782740000000000
B	7.441380000000000	7.479880000000000	7.210920000000000
B	16.459959999999999	12.436030000000001	7.465290000000000
B	15.976470000000001	9.051819999999999	7.038260000000000
B	14.096159999999999	14.879810000000001	6.903380000000000
B	5.720680000000000	12.926209999999999	7.101510000000000
B	5.483940000000000	9.212830000000000	7.180340000000000
H	8.328580000000001	16.660080000000001	5.875100000000000
H	10.001070000000000	17.673790000000000	6.550150000000000
H	6.205780000000000	13.786149999999999	8.027390000000000
H	6.774170000000000	15.422850000000000	7.026640000000000
H	11.708530000000000	4.328960000000000	6.648080000000000
H	13.367630000000000	5.308610000000000	5.898150000000000
H	14.876650000000000	6.586210000000000	6.975220000000000
H	15.603550000000000	8.220810000000000	6.044770000000000
H	8.974940000000000	4.895750000000000	7.941360000000000
H	8.692410000000001	5.141010000000000	5.912000000000000
H	13.686360000000001	15.635360000000000	5.871840000000000
H	12.926170000000001	17.327459999999999	6.697910000000000
H	6.225740000000000	7.698810000000000	7.284410000000000
H	7.672230000000000	6.264870000000000	7.302320000000000
H	16.495830000000002	13.478050000000000	8.058940000000000
H	17.496559999999999	11.876720000000001	7.215190000000000
H	15.502520000000001	8.206239999999999	7.970990000000000
H	17.168469999999999	8.972149999999999	7.096810000000000
H	13.649120000000000	15.776710000000000	7.794880000000000
H	15.282539999999999	15.008570000000001	6.901970000000000
H	4.528020000000000	12.994850000000000	7.183640000000000
H	6.069280000000000	13.776630000000001	6.103210000000000
H	4.918360000000000	8.870870000000000	6.168810000000000
H	4.925440000000000	9.002210000000000	8.230750000000000
O	10.861090000000001	11.004350000000001	9.148740000000000
N	10.746930000000001	13.059049999999999	6.913220000000000
N	10.944240000000001	8.935670000000000	6.920610000000000
N	12.872629999999999	11.101139999999999	6.953740000000000
N	8.884690000000001	10.972270000000000	6.951970000000000
Cu	10.867680000000000	11.022819999999999	7.214910000000000

Transition Metal: Cu; Functional Group: BH2; Adsorbate: OH

C	10.150340000000000	15.339330000000000	6.629410000000000
C	9.670690000000000	13.940519999999999	6.757260000000000
C	8.340130000000000	13.451060000000000	6.830760000000000
C	11.592090000000001	6.668610000000000	6.681860000000000
C	12.049329999999999	8.081640000000000	6.736130000000000
C	13.353710000000000	8.590830000000000	6.788380000000000
C	10.198650000000001	6.719510000000000	6.819870000000000
C	9.850770000000001	8.133640000000000	6.884700000000000
C	11.549239999999999	15.242830000000000	6.697460000000000
C	8.496380000000000	8.549070000000000	6.986290000000000
C	15.130860000000000	11.726200000000000	7.014090000000000
C	11.878250000000000	13.847670000000001	6.816340000000000
C	13.726270000000000	12.195589999999999	6.942840000000000
C	15.047129999999999	10.332890000000001	6.926610000000000
C	13.646160000000000	9.984010000000000	6.858820000000000
C	13.254020000000001	13.517920000000000	6.876300000000000
C	6.672860000000000	11.669040000000001	6.991110000000000
C	8.068569999999999	12.076589999999999	6.900810000000000
C	6.660740000000000	10.280480000000001	7.031980000000000
C	8.081849999999999	9.896910000000000	6.970400000000000
B	9.424239999999999	16.647160000000000	6.257040000000000
B	6.943240000000000	14.243100000000000	6.900910000000000
B	12.302429999999999	5.356540000000000	6.309290000000000
B	14.732440000000000	7.775380000000000	6.845900000000000
B	9.114910000000000	5.574680000000000	6.836240000000000
B	12.842409999999999	16.141439999999999	6.632550000000000
B	7.439480000000000	7.495670000000000	7.105180000000000
B	16.444870000000002	12.441110000000000	7.393400000000000
B	15.973190000000001	9.060020000000000	6.943560000000000
B	14.103730000000001	14.878060000000000	6.769010000000000
B	5.728590000000000	12.921099999999999	7.008060000000000
B	5.512340000000000	9.205730000000001	7.105850000000000
H	10.610230000000000	11.837540000000001	9.462759999999999
H	8.318470000000000	16.675830000000001	5.792280000000000
H	10.027170000000000	17.682820000000000	6.380210000000000
H	6.201000000000000	13.798080000000001	7.923790000000000
H	6.766040000000000	15.423340000000000	6.904840000000000
H	11.700749999999999	4.326420000000000	6.493250000000000
H	13.380549999999999	5.301880000000000	5.785470000000000
H	14.882529999999999	6.592170000000000	6.845120000000000
H	15.608840000000001	8.239470000000001	5.938400000000000
H	8.973910000000000	4.900990000000000	7.828710000000000
H	8.695050000000000	5.128810000000000	5.795240000000000
H	13.692080000000001	15.617260000000000	5.726140000000000
H	12.946130000000000	17.328420000000001	6.526210000000000
H	6.223360000000000	7.727610000000000	7.185640000000000
H	7.652070000000000	6.278580000000000	7.170200000000000
H	16.472940000000001	13.482790000000000	7.988190000000000
H	17.484950000000001	11.883660000000001	7.154080000000000
H	15.499620000000000	8.201320000000001	7.864000000000000
H	17.165559999999999	8.985840000000000	7.004880000000000
H	13.668340000000001	15.794409999999999	7.645450000000000
H	15.291180000000001	15.000260000000001	6.757100000000000
H	4.534780000000000	12.981370000000000	7.080510000000000
H	6.076100000000000	13.760830000000000	6.000540000000000
H	4.928400000000000	8.885669999999999	6.096780000000000
H	4.956440000000000	8.996290000000000	8.158510000000000
O	10.876640000000000	10.959410000000000	9.122600000000000
N	10.747900000000000	13.075450000000000	6.852520000000000
N	10.948700000000001	8.929600000000001	6.824770000000000
N	12.862970000000001	11.103080000000000	6.854620000000000
N	8.904880000000000	10.981150000000000	6.873230000000000
Cu	10.873279999999999	11.018850000000000	7.085530000000000

Transition Metal: Cu; Functional Group: BH2; Adsorbate: OOH

Cu	10.867680000000000	11.022819999999999	7.214910000000000
C	10.144180000000000	15.324870000000001	6.745290000000000
C	9.666119999999999	13.923670000000000	6.844590000000000
C	8.335010000000000	13.440939999999999	6.918410000000000
C	11.588749999999999	6.673400000000000	6.812400000000000
C	12.047140000000001	8.085410000000000	6.851740000000000
C	13.353710000000000	8.589580000000000	6.897630000000000
C	10.194780000000000	6.725360000000000	6.945460000000000
C	9.845030000000000	8.138400000000001	6.991690000000000
C	11.541420000000000	15.231619999999999	6.823000000000000
C	8.486490000000000	8.544810000000000	7.078200000000000
C	15.140820000000000	11.722670000000001	7.099040000000000
C	11.875700000000000	13.833959999999999	6.914840000000000
C	13.735590000000000	12.193130000000000	7.036600000000000
C	15.055380000000000	10.328550000000000	7.012880000000000
C	13.654080000000000	9.981460000000000	6.953960000000000
C	13.254120000000000	13.513010000000000	6.979280000000000
C	6.655860000000000	11.666779999999999	7.064550000000000
C	8.052809999999999	12.067539999999999	6.976450000000000
C	6.639440000000000	10.277369999999999	7.106350000000000
C	8.060630000000000	9.889239999999999	7.047430000000000
B	9.416350000000000	16.634380000000000	6.381340000000000
B	6.943740000000000	14.241569999999999	7.005910000000000
B	12.299700000000000	5.360600000000000	6.442830000000000
B	14.730140000000000	7.769640000000000	6.961060000000000
B	9.104730000000000	5.584810000000000	6.957470000000000
B	12.829590000000000	16.138290000000001	6.782740000000000
B	7.441380000000000	7.479880000000000	7.210920000000000
B	16.459959999999999	12.436030000000001	7.465290000000000
B	15.976470000000001	9.051819999999999	7.038260000000000
B	14.096159999999999	14.879810000000001	6.903380000000000
B	5.720680000000000	12.926209999999999	7.101510000000000
B	5.483940000000000	9.212830000000000	7.180340000000000
H	8.328580000000001	16.660080000000001	5.875100000000000
H	10.001070000000000	17.673790000000000	6.550150000000000
H	6.205780000000000	13.786149999999999	8.027390000000000
H	6.774170000000000	15.422850000000000	7.026640000000000
H	11.708530000000000	4.328960000000000	6.648080000000000
H	13.367630000000000	5.308610000000000	5.898150000000000
H	14.876650000000000	6.586210000000000	6.975220000000000
H	15.603550000000000	8.220810000000000	6.044770000000000
H	8.974940000000000	4.895750000000000	7.941360000000000
H	8.692410000000001	5.141010000000000	5.912000000000000
H	13.686360000000001	15.635360000000000	5.871840000000000
H	12.926170000000001	17.327459999999999	6.697910000000000
H	6.225740000000000	7.698810000000000	7.284410000000000
H	7.672230000000000	6.264870000000000	7.302320000000000
H	16.495830000000002	13.478050000000000	8.058940000000000
H	17.496559999999999	11.876720000000001	7.215190000000000
H	15.502520000000001	8.206239999999999	7.970990000000000
H	17.168469999999999	8.972149999999999	7.096810000000000
H	13.649120000000000	15.776710000000000	7.794880000000000
H	15.282539999999999	15.008570000000001	6.901970000000000
H	4.528020000000000	12.994850000000000	7.183640000000000
H	6.069280000000000	13.776630000000001	6.103210000000000
H	4.918360000000000	8.870870000000000	6.168810000000000
H	4.925440000000000	9.002210000000000	8.230750000000000
N	10.746930000000001	13.059049999999999	6.913220000000000
N	10.944240000000001	8.935670000000000	6.920610000000000
N	12.872629999999999	11.101139999999999	6.953740000000000
N	8.884690000000001	10.972270000000000	6.951970000000000
O	10.859055440206641	10.998647675359127	9.745779873322180
H	10.826696436024907	9.208737375113882	9.193204182228090
O	11.061790951522330	9.657723405638993	10.056656212592642

Transition Metal: Cu; Functional Group: CH3; Adsorbate: Clean

H	9.110260000000000	16.242920000000002	8.992940000000001
H	10.555709999999999	17.165820000000000	8.572110000000000
H	9.211240000000000	17.075720000000000	7.428910000000000
H	6.603740000000000	14.216060000000001	7.156750000000000
H	7.194510000000000	14.878040000000000	8.690110000000001
H	7.848860000000000	15.443960000000001	7.143890000000000
H	12.499000000000001	5.613410000000000	9.644399999999999
H	11.967680000000000	4.762340000000000	8.185840000000001
H	13.446099999999999	5.724200000000000	8.152100000000001
H	14.815379999999999	8.713419999999999	9.983390000000000
H	13.552759999999999	7.498990000000000	10.149260000000000
H	14.827410000000000	7.282760000000000	8.938840000000001
H	9.466590000000000	5.289980000000000	6.229990000000000
H	10.028890000000001	4.718120000000000	7.808670000000000
H	8.545809999999999	5.666680000000000	7.694930000000000
H	12.273830000000000	17.255310000000001	7.550840000000000
H	13.667330000000000	16.176089999999999	7.374240000000000
H	12.787929999999999	16.740700000000000	5.942940000000000
H	8.415229999999999	7.056370000000000	5.355200000000000
H	7.161390000000000	7.027590000000000	6.605710000000000
H	7.134440000000000	8.265290000000000	5.338530000000000
H	16.433479999999999	13.374359999999999	6.964750000000000
H	17.328040000000001	11.853859999999999	6.964540000000000
H	16.525620000000000	12.405650000000000	5.485480000000000
H	16.660409999999999	9.605790000000001	9.108060000000000
H	16.274529999999999	8.524010000000001	7.759730000000000
H	17.278540000000000	9.948490000000000	7.485210000000000
H	14.947089999999999	14.764570000000001	6.087360000000000
H	14.719790000000000	13.525100000000000	4.843220000000000
H	13.560779999999999	14.843620000000000	4.985860000000000
H	4.847200000000000	11.588900000000001	8.685430000000000
H	5.799810000000000	13.029080000000000	9.051100000000000
H	4.973420000000000	12.882190000000000	7.487850000000000
H	5.783080000000000	8.419790000000001	7.757740000000000
H	4.724860000000000	9.840100000000000	7.756070000000000
H	5.271410000000000	9.150440000000000	6.226920000000000
C	10.436600000000000	15.258039999999999	7.577630000000000
C	9.926550000000001	13.883520000000001	7.553880000000000
C	8.571529999999999	13.471240000000000	7.684670000000000
C	11.613680000000000	6.890670000000000	8.104870000000000
C	12.009630000000000	8.301890000000000	8.116560000000000
C	13.290240000000001	8.814539999999999	8.455909999999999
C	10.369500000000000	6.827890000000000	7.495540000000000
C	9.965579999999999	8.207839999999999	7.215510000000000
C	11.734590000000001	15.215070000000001	7.092620000000000
C	8.680830000000000	8.641060000000000	6.798890000000000
C	15.184450000000000	11.597939999999999	7.010990000000000
C	12.057050000000000	13.806940000000001	6.878770000000000
C	13.787430000000001	12.021789999999999	6.887040000000000
C	15.178060000000000	10.398149999999999	7.706850000000000
C	13.774229999999999	10.044840000000001	7.931200000000000
C	13.323520000000000	13.296180000000000	6.475240000000000
C	6.762330000000000	11.624200000000000	7.697590000000000
C	8.142310000000000	12.116820000000001	7.624890000000000
C	6.785450000000000	10.297090000000001	7.298400000000000
C	8.188400000000000	9.943569999999999	7.093360000000000
C	9.788629999999999	16.489580000000000	8.165749999999999
C	7.501750000000000	14.556509999999999	7.680210000000000
C	12.420030000000001	5.695300000000000	8.547390000000000
C	14.172370000000001	8.029800000000000	9.415970000000000
C	9.564959999999999	5.568800000000000	7.292180000000000
C	12.663060000000000	16.397639999999999	6.984240000000000
C	7.796960000000000	7.693650000000000	6.000190000000000
C	16.422809999999998	12.342860000000000	6.581210000000000
C	16.402509999999999	9.580690000000001	8.035890000000000
C	14.188810000000000	14.157510000000000	5.566720000000000

C	5.542370000000000	12.322609999999999	8.251260000000000
C	5.589530000000000	9.380530000000000	7.257640000000000
Cu	10.972810000000001	11.046580000000001	7.369910000000000
N	10.970490000000000	13.032100000000000	7.222410000000000
N	10.985200000000001	9.061030000000001	7.586290000000000
N	12.970820000000000	11.044820000000000	7.424470000000000
N	8.978320000000000	11.044890000000001	7.346710000000000

Transition Metal: Cu; Functional Group: CH3; Adsorbate: O

H	9.094420000000000	16.233640000000001	8.996050000000000
H	10.543220000000000	17.161760000000001	8.598470000000001
H	9.213080000000000	17.076860000000000	7.438880000000000
H	6.617650000000000	14.206300000000001	7.089940000000000
H	7.183480000000000	14.885920000000000	8.625610000000000
H	7.864040000000000	15.435790000000001	7.084460000000000
H	12.491170000000000	5.634430000000000	9.674480000000001
H	11.950310000000000	4.762710000000000	8.231590000000001
H	13.433330000000000	5.716040000000000	8.176220000000001
H	14.806369999999999	8.734120000000001	9.973360000000000
H	13.541280000000000	7.521280000000000	10.147500000000001
H	14.818440000000001	7.293720000000000	8.941540000000000
H	9.448910000000000	5.283970000000000	6.260800000000000
H	10.009670000000000	4.717550000000000	7.842800000000000
H	8.531350000000000	5.672760000000000	7.724890000000000
H	12.293650000000000	17.248790000000000	7.623220000000000
H	13.680400000000001	16.165310000000002	7.425150000000000
H	12.805030000000000	16.763510000000000	6.004940000000000
H	8.420460000000000	7.068350000000000	5.348640000000000
H	7.160820000000000	7.030020000000000	6.595250000000000
H	7.138040000000000	8.277600000000000	5.335800000000000
H	16.442720000000001	13.380400000000000	6.974010000000000
H	17.335930000000001	11.859170000000001	6.963370000000000
H	16.528430000000000	12.419580000000000	5.489150000000000
H	16.658400000000000	9.603930000000000	9.102959999999999
H	16.273859999999999	8.524609999999999	7.751130000000000
H	17.280210000000000	9.948060000000000	7.481540000000000
H	14.949249999999999	14.768030000000000	6.082650000000000
H	14.703430000000001	13.532750000000000	4.835620000000000
H	13.550240000000001	14.856109999999999	4.996150000000000
H	4.847450000000000	11.606820000000001	8.684680000000000
H	5.804870000000000	13.046970000000000	9.037920000000000
H	4.978260000000000	12.888949999999999	7.476040000000000
H	5.792850000000000	8.416779999999999	7.791780000000000
H	4.729440000000000	9.833360000000001	7.799410000000000
H	5.260150000000000	9.141629999999999	6.264650000000000
C	10.439030000000001	15.261030000000000	7.589530000000000
C	9.931390000000000	13.885730000000001	7.550070000000000
C	8.575450000000000	13.470240000000000	7.659910000000000
C	11.606140000000000	6.890890000000000	8.118410000000001
C	12.004330000000000	8.303319999999999	8.111350000000000
C	13.284580000000000	8.821730000000001	8.444870000000000
C	10.360099999999999	6.823830000000000	7.513450000000000
C	9.959820000000001	8.201940000000000	7.221940000000000
C	11.743240000000000	15.221719999999999	7.120610000000000
C	8.676940000000000	8.639310000000000	6.802640000000000
C	15.192060000000000	11.604830000000000	7.010840000000000
C	12.064520000000000	13.815480000000001	6.894800000000000
C	13.796469999999999	12.031090000000001	6.888040000000000
C	15.180880000000000	10.401000000000000	7.699480000000000
C	13.773650000000000	10.050300000000000	7.917570000000000
C	13.329230000000001	13.304890000000000	6.480260000000000
C	6.761840000000000	11.627150000000000	7.696090000000000
C	8.143520000000001	12.115539999999999	7.616410000000000
C	6.782250000000000	10.295240000000000	7.312540000000000
C	8.183930000000000	9.940569999999999	7.105060000000000
C	9.782200000000000	16.486820000000002	8.178720000000000
C	7.506440000000000	14.554489999999999	7.624180000000000
C	12.408780000000000	5.699250000000000	8.576510000000001
C	14.163940000000000	8.045210000000001	9.412140000000001
C	9.549620000000001	5.567450000000000	7.321560000000000
C	12.677930000000000	16.400780000000001	7.039030000000000
C	7.797420000000000	7.699630000000000	5.994710000000000
C	16.430270000000000	12.351020000000000	6.584820000000000
C	16.402590000000000	9.580510000000000	8.030139999999999
C	14.184089999999999	14.166420000000000	5.566000000000000

C	5.544960000000000	12.334440000000001	8.244400000000001
C	5.589130000000000	9.375100000000000	7.291120000000000
O	11.032130000000000	10.820860000000000	5.126520000000000
Cu	10.976310000000000	11.026880000000000	7.111130000000000
N	10.980940000000000	13.039640000000000	7.233070000000000
N	10.976070000000000	9.056170000000000	7.585350000000000
N	12.977010000000000	11.059060000000001	7.424110000000000
N	8.975059999999999	11.037620000000000	7.360860000000000

Transition Metal: Cu; Functional Group: CH3; Adsorbate: OH

H	10.405960000000000	11.521220000000000	4.718100000000000
H	9.098310000000000	16.231729999999999	9.021780000000000
H	10.547160000000000	17.163150000000002	8.630830000000000
H	9.217860000000000	17.084969999999998	7.469910000000000
H	6.622710000000000	14.216300000000000	7.106160000000000
H	7.190670000000000	14.879949999999999	8.647320000000001
H	7.868830000000000	15.447229999999999	7.111900000000000
H	12.495660000000001	5.643810000000000	9.689750000000000
H	11.945740000000001	4.767830000000000	8.253220000000001
H	13.433870000000001	5.712520000000000	8.187989999999999
H	14.818840000000000	8.739170000000000	9.975059999999999
H	13.552580000000001	7.527460000000000	10.154940000000000
H	14.822810000000000	7.299710000000000	8.941739999999999
H	9.456239999999999	5.293580000000000	6.264360000000000
H	10.015129999999999	4.722790000000000	7.845230000000000
H	8.537739999999999	5.679940000000000	7.729250000000000
H	12.305619999999999	17.249790000000001	7.682050000000000
H	13.691390000000000	16.168920000000000	7.464060000000000
H	12.814930000000000	16.792410000000000	6.055090000000000
H	8.441580000000000	7.084130000000000	5.334710000000000
H	7.183010000000000	7.031530000000000	6.582530000000000
H	7.151820000000000	8.286870000000000	5.330740000000000
H	16.458520000000000	13.379949999999999	6.987490000000000
H	17.344290000000001	11.854820000000000	6.962180000000000
H	16.532029999999999	12.427270000000000	5.495970000000000
H	16.669550000000001	9.602969999999999	9.100490000000001
H	16.277500000000000	8.525679999999999	7.748910000000000
H	17.284540000000000	9.947880000000000	7.476750000000000
H	14.966030000000000	14.773740000000000	6.117670000000000
H	14.713369999999999	13.554930000000001	4.855940000000000
H	13.567270000000001	14.883530000000000	5.032820000000000
H	4.851900000000000	11.603540000000001	8.673430000000000
H	5.807020000000000	13.042870000000001	9.037280000000001
H	4.982570000000000	12.893280000000001	7.472750000000000
H	5.802480000000000	8.420620000000000	7.779760000000000
H	4.737470000000000	9.835649999999999	7.786830000000000
H	5.269560000000000	9.144940000000000	6.252850000000000
C	10.445380000000000	15.268879999999999	7.610040000000000
C	9.937640000000000	13.894000000000000	7.557070000000000
C	8.581820000000000	13.475450000000000	7.666140000000000
C	11.611300000000000	6.895570000000000	8.129569999999999
C	12.009600000000001	8.309220000000000	8.120540000000000
C	13.289910000000001	8.828780000000000	8.452980000000000
C	10.367580000000000	6.829330000000000	7.520680000000000
C	9.970800000000001	8.209009999999999	7.226270000000000
C	11.752500000000000	15.232360000000000	7.147750000000000
C	8.690270000000000	8.646850000000001	6.798050000000000
C	15.199820000000001	11.610070000000000	7.019470000000000
C	12.072170000000000	13.827240000000000	6.909940000000000
C	13.803850000000001	12.038910000000000	6.901650000000000
C	15.187550000000000	10.404669999999999	7.704200000000000
C	13.778940000000000	10.057710000000000	7.924060000000000
C	13.338690000000000	13.315110000000001	6.498250000000000
C	6.767860000000000	11.631489999999999	7.688490000000000
C	8.149590000000000	12.120609999999999	7.612790000000000
C	6.790380000000000	10.300010000000000	7.302890000000000
C	8.193049999999999	9.947770000000000	7.097740000000000
C	9.786849999999999	16.490490000000001	8.206490000000001
C	7.512330000000000	14.559650000000000	7.641970000000000
C	12.410600000000001	5.703330000000000	8.591860000000000
C	14.171980000000000	8.051720000000000	9.416990000000000
C	9.556020000000000	5.574190000000000	7.325780000000000
C	12.688800000000001	16.411709999999999	7.082930000000000
C	7.815140000000000	7.707950000000000	5.984910000000000
C	16.439029999999999	12.353220000000000	6.591590000000000
C	16.408770000000001	9.581000000000000	8.028790000000001

C	14.197190000000001	14.182910000000000	5.593760000000000
C	5.549130000000000	12.334949999999999	8.238700000000000
C	5.598030000000000	9.378679999999999	7.279220000000000
O	11.014430000000001	10.842930000000001	5.070960000000000
Cu	10.986570000000000	11.030720000000001	7.109160000000000
N	10.985939999999999	13.049410000000000	7.231340000000000
N	10.985780000000000	9.062210000000000	7.589390000000000
N	12.982839999999999	11.067280000000000	7.434840000000000
N	8.983459999999999	11.044549999999999	7.354880000000000

Transition Metal: Cu; Functional Group: CH3; Adsorbate: OOH

Cu	10.976310000000000	11.026880000000000	7.111130000000000
H	9.094420000000000	16.233640000000001	8.996050000000000
H	10.543220000000000	17.161760000000001	8.598470000000001
H	9.213080000000000	17.076860000000000	7.438880000000000
H	6.617650000000000	14.206300000000001	7.089940000000000
H	7.183480000000000	14.885920000000000	8.625610000000000
H	7.864040000000000	15.435790000000001	7.084460000000000
H	12.491170000000000	5.634430000000000	9.674480000000001
H	11.950310000000000	4.762710000000000	8.231590000000001
H	13.433330000000000	5.716040000000000	8.176220000000001
H	14.806369999999999	8.734120000000001	9.973360000000000
H	13.541280000000000	7.521280000000000	10.147500000000001
H	14.818440000000001	7.293720000000000	8.941540000000000
H	9.448910000000000	5.283970000000000	6.260800000000000
H	10.009670000000000	4.717550000000000	7.842800000000000
H	8.531350000000000	5.672760000000000	7.724890000000000
H	12.293650000000000	17.248790000000000	7.623220000000000
H	13.680400000000001	16.165310000000002	7.425150000000000
H	12.805030000000000	16.763510000000000	6.004940000000000
H	8.420460000000000	7.068350000000000	5.348640000000000
H	7.160820000000000	7.030020000000000	6.595250000000000
H	7.138040000000000	8.277600000000000	5.335800000000000
H	16.442720000000001	13.380400000000000	6.974010000000000
H	17.335930000000001	11.859170000000001	6.963370000000000
H	16.528430000000000	12.419580000000000	5.489150000000000
H	16.658400000000000	9.603930000000000	9.102959999999999
H	16.273859999999999	8.524609999999999	7.751130000000000
H	17.280210000000000	9.948060000000000	7.481540000000000
H	14.949249999999999	14.768030000000000	6.082650000000000
H	14.703430000000001	13.532750000000000	4.835620000000000
H	13.550240000000001	14.856109999999999	4.996150000000000
H	4.847450000000000	11.606820000000001	8.684680000000000
H	5.804870000000000	13.046970000000000	9.037920000000000
H	4.978260000000000	12.888949999999999	7.476040000000000
H	5.792850000000000	8.416779999999999	7.791780000000000
H	4.729440000000000	9.833360000000001	7.799410000000000
H	5.260150000000000	9.141629999999999	6.264650000000000
C	10.439030000000001	15.261030000000000	7.589530000000000
C	9.931390000000000	13.885730000000001	7.550070000000000
C	8.575450000000000	13.470240000000000	7.659910000000000
C	11.606140000000000	6.890890000000000	8.118410000000001
C	12.004330000000000	8.303319999999999	8.111350000000000
C	13.284580000000000	8.821730000000001	8.444870000000000
C	10.360099999999999	6.823830000000000	7.513450000000000
C	9.959820000000001	8.201940000000000	7.221940000000000
C	11.743240000000000	15.221719999999999	7.120610000000000
C	8.676940000000000	8.639310000000000	6.802640000000000
C	15.192060000000000	11.604830000000000	7.010840000000000
C	12.064520000000000	13.815480000000001	6.894800000000000
C	13.796469999999999	12.031090000000001	6.888040000000000
C	15.180880000000000	10.401000000000000	7.699480000000000
C	13.773650000000000	10.050300000000000	7.917570000000000
C	13.329230000000001	13.304890000000000	6.480260000000000
C	6.761840000000000	11.627150000000000	7.696090000000000
C	8.143520000000001	12.115539999999999	7.616410000000000
C	6.782250000000000	10.295240000000000	7.312540000000000
C	8.183930000000000	9.940569999999999	7.105060000000000
C	9.782200000000000	16.486820000000002	8.178720000000000
C	7.506440000000000	14.554489999999999	7.624180000000000
C	12.408780000000000	5.699250000000000	8.576510000000001
C	14.163940000000000	8.045210000000001	9.412140000000001
C	9.549620000000001	5.567450000000000	7.321560000000000
C	12.677930000000000	16.400780000000001	7.039030000000000
C	7.797420000000000	7.699630000000000	5.994710000000000
C	16.430270000000000	12.351020000000000	6.584820000000000
C	16.402590000000000	9.580510000000000	8.030139999999999

C	14.184089999999999	14.166420000000000	5.566000000000000
C	5.544960000000000	12.334440000000001	8.244400000000001
C	5.589130000000000	9.375100000000000	7.291120000000000
N	10.980940000000000	13.039640000000000	7.233070000000000
N	10.976070000000000	9.056170000000000	7.585350000000000
N	12.977010000000000	11.059060000000001	7.424110000000000
N	8.975059999999999	11.037620000000000	7.360860000000000
O	11.047089810749135	10.765646452695508	4.594642715678256
H	10.098949002683538	12.343659587488414	4.942593052602282
O	10.558666070821193	11.982659950073089	4.129729734071268

Transition Metal: Cu; Functional Group: F; Adsorbate: Clean

Cu	0.000000000000000	-0.000001081314558	-0.003532568066820
C	0.685023738038704	4.261555580147216	-0.002246757494202
C	1.109615936585288	2.880828519134994	-0.003440471922784
C	2.433469288886218	2.433342468703180	-0.001785754459454
C	-0.685030913595654	-4.261500059548542	-0.001728549371425
C	-1.109645379590656	-2.880810070076695	-0.002012688097288
C	-2.433472550436033	-2.433291521675812	-0.001846477195606
C	0.685030913595650	-4.261500059548542	-0.001728549371425
C	1.109645379590656	-2.880810070076695	-0.002012688097288
C	-0.685023738038716	4.261555580147216	-0.002246757494202
C	2.433472550436034	-2.433291521675812	-0.001846477195606
C	-4.262036697967133	0.685056736519928	0.002400420755898
C	-1.109615936585289	2.880828519134994	-0.003440471922784
C	-2.881278165124950	1.109558266002182	0.000713497074318
C	-4.261993800907307	-0.685034315322245	0.001881845335842
C	-2.881264729610258	-1.109569405250852	0.000365483522012
C	-2.433469288886226	2.433342468703180	-0.001785754459454
C	4.262036697967138	0.685056736519928	0.002400420755898
C	2.881278165124946	1.109558266002182	0.000713497074318
C	4.261993800907312	-0.685034315322245	0.001881845335842
C	2.881264729610268	-1.109569405250852	0.000365483522012
N	0.000000000000000	2.048761589690984	-0.004988943557322
N	0.000000000000000	-2.048698263204734	-0.002636107171396
N	-2.049161707023394	0.000005325405494	0.000020873766232
N	2.049161707023392	0.000005325405494	0.000020873766232
F	5.349275779044937	-1.477030777758735	0.001467112108568
F	-5.349360148185420	1.476985313851014	0.002436438676490
F	-5.349275779044927	-1.477030777758735	0.001467112108568
F	-1.476996135696751	5.348864318536288	-0.000312429686041
F	1.476996135696758	5.348864318536288	-0.000312429686041
F	5.349360148185416	1.476985313851014	0.002436438676490
F	-1.476962685313204	-5.348820529616965	-0.000782382582017
F	1.476962685313202	-5.348820529616965	-0.000782382582017
F	-3.397520244577109	3.397561774880284	-0.000687182324812
F	3.397520244577106	3.397561774880284	-0.000687182324812
F	-3.397590858997855	-3.397522746516465	-0.002019168708206
F	3.397590858997850	-3.397522746516465	-0.002019168708206

Transition Metal: Cu; Functional Group: F; Adsorbate: O

Cu	0.000000000000000	-0.028464344624986	0.257796608745106
C	0.685399149749460	4.282056856095734	-0.014003070338838
C	1.105719372451950	2.897869002276006	-0.038602777517085
C	2.426916747914000	2.435481397053012	-0.009813259973090
C	-0.685701055836820	-4.277398046322396	-0.010684318542175
C	-1.109006500193253	-2.895794318852413	-0.034394279328037
C	-2.430978201433916	-2.437585452329952	-0.006613908573144
C	0.685701055836830	-4.277398046322396	-0.010684318542175
C	1.109006500193248	-2.895794318852413	-0.034394279328037
C	-0.685399149749461	4.282056856095734	-0.014003070338838
C	2.430978201433916	-2.437585452329952	-0.006613908573144
C	-4.259914074785847	0.685919032442102	0.009489768790898
C	-1.105719372451951	2.897869002276006	-0.038602777517085
C	-2.877790723457402	1.108559280128118	0.007678891596770
C	-4.262259589558184	-0.685857957129034	0.009693437177812
C	-2.881926515922203	-1.111386167105639	0.008613825521814
C	-2.426916747914003	2.435481397053012	-0.009813259973090
C	4.259914074785848	0.685919032442102	0.009489768790898
C	2.877790723457406	1.108559280128118	0.007678891596770
C	4.262259589558184	-0.685857957129034	0.009693437177812
C	2.881926515922206	-1.111386167105639	0.008613825521814
N	0.000000000000000	2.070990056882404	-0.081145388835910
N	0.000000000000000	-2.069618791869893	-0.081161358138658
N	-2.053073285874540	-0.003288386708029	-0.001125176324795
N	2.053073285874534	-0.003288386708029	-0.001125176324795
F	5.349967930894673	-1.475423050417028	-0.004693756855115
F	-5.346012159322191	1.477432335947724	-0.005072261590289
F	-5.349967930894667	-1.475423050417028	-0.004693756855115
F	-1.479413266988601	5.367147025614244	0.000077861230600
F	1.479413266988612	5.367147025614244	0.000077861230600
F	5.346012159322182	1.477432335947724	-0.005072261590289
F	-1.478464260751473	-5.362688040942167	-0.000100580687122
F	1.478464260751476	-5.362688040942167	-0.000100580687122
F	-3.393849999574684	3.391836070205274	0.009672041016506
F	3.393849999574686	3.391836070205274	0.009672041016506
F	-3.395827835193479	-3.395949313364873	0.013948245039056
F	3.395827835193482	-3.395949313364873	0.013948245039056
O	0.000000000000000	-0.008387453568581	2.205238776941336

Transition Metal: Cu; Functional Group: F; Adsorbate: OH

Cu	0.000000000000000	0.000968962615088	0.248456257717636
C	0.685783033693180	4.263870116915117	-0.004946779399756
C	1.110257998358962	2.883073685681590	-0.004049618670772
C	2.435786453333688	2.430185308479272	-0.016102465362560
C	-0.685412463490181	-4.265092620108726	-0.003479713217260
C	-1.107424793670887	-2.882230587840951	-0.008591733820044
C	-2.432996557805446	-2.429359535107412	-0.011922918038678
C	0.685412463490186	-4.265092620108726	-0.003479713217260
C	1.107424793670894	-2.882230587840951	-0.008591733820044
C	-0.685783033693188	4.263870116915117	-0.004946779399756
C	2.432996557805450	-2.429359535107412	-0.011922918038678
C	-4.275890056311402	0.684707332609128	-0.010918269657740
C	-1.110257998358957	2.883073685681590	-0.004049618670772
C	-2.893367231995381	1.107425213606248	-0.034808095113895
C	-4.274620583866472	-0.686043884746844	-0.008871239455388
C	-2.891326164120638	-1.106741175139330	-0.031279483532982
C	-2.435786453333691	2.430185308479272	-0.016102465362560
C	4.275890056311392	0.684707332609128	-0.010918269657740
C	2.893367231995380	1.107425213606248	-0.034808095113895
C	4.274620583866464	-0.686043884746844	-0.008871239455388
C	2.891326164120644	-1.106741175139330	-0.031279483532982
N	0.000000000000000	2.054669293729136	-0.009235133594846
N	0.000000000000000	-2.055413198804096	-0.022818090513518
N	-2.065278446308167	0.000693127800050	-0.071597380071129
N	2.065278446308172	0.000693127800050	-0.071597380071129
F	5.359936464849048	-1.479407628924193	0.001045765483168
F	-5.362179455095591	1.477189050830220	-0.000726548222772
F	-5.359936464849046	-1.479407628924193	0.001045765483168
F	-1.476169793956764	5.351418107364934	-0.016179637888559
F	1.476169793956760	5.351418107364934	-0.016179637888559
F	5.362179455095580	1.477189050830220	-0.000726548222772
F	-1.477127586525732	-5.351692023447971	-0.010153498074260
F	1.477127586525730	-5.351692023447971	-0.010153498074260
F	-3.395117404349495	3.394871989887766	0.001044729860032
F	3.395117404349492	3.394871989887766	0.001044729860032
F	-3.392177366419588	-3.393037334404418	0.009195150295048
F	3.392177366419586	-3.393037334404418	0.009195150295048
H	0.000000000000000	0.893963891965210	2.601176048467192
O	0.000000000000000	-0.016727236414059	2.246734387698050

Transition Metal: Cu; Functional Group: F; Adsorbate: OOH

Cu	-0.003032493074154	-0.002384443450818	0.008714081361208
C	0.682130696888522	4.263630592376518	-0.028853154313683
C	1.106316089053390	2.882304206832020	-0.042192684963678
C	2.429700806340438	2.431992893957404	-0.040855599719268
C	-0.687891703881427	-4.266687128429291	-0.047066739826938
C	-1.111659628707596	-2.885056903945543	-0.064082090833356
C	-2.435204628531423	-2.434042181870979	-0.060761669666294
C	0.682038583920520	-4.266234253327863	-0.039816077127764
C	1.105023610365774	-2.884210607229786	-0.053819286315026
C	-0.687869250078080	4.263803626635430	-0.033267214495964
C	2.428545252458444	-2.432865580033024	-0.044303833497170
C	-4.267050907464094	0.683398915608468	-0.042709152637595
C	-1.112296451608291	2.882600738893114	-0.049357543796044
C	-2.885792899399199	1.107541961068056	-0.063779544269046
C	-4.266753747896301	-0.686669333352818	-0.044438109525775
C	-2.885337003547686	-1.110180189655626	-0.066810321926484
C	-2.435538482507546	2.431624487942828	-0.052831441900504
C	4.261470195854890	0.684107591586364	-0.032573171275608
C	2.880094526617770	1.108025124370634	-0.052159287594979
C	4.261058021214854	-0.685867096263962	-0.032449239603988
C	2.879341686264524	-1.109085573843835	-0.052146209524848
N	-0.002961391345824	2.052547755106904	-0.055741917916616
N	-0.003520588990044	-2.055494197674093	-0.071567428988804
N	-2.056009859918284	-0.001095155200750	-0.085364864489531
N	2.050398237301970	-0.000149183564986	-0.071922181512182
F	5.348054160309236	-1.478652555453305	-0.014126087152442
F	-5.354646566627324	1.476050970584186	-0.019000739324694
F	-5.353965410605191	-1.479234806212609	-0.022977896152864
F	-1.480700503087167	5.351333736436454	-0.022444357756774
F	1.474627274667456	5.350978273978482	-0.012925362160134
F	5.348819895487438	1.476589946193438	-0.013342562037430
F	-1.480748439235551	-5.353773730829833	-0.036223322036496
F	1.475253785699640	-5.352822654372432	-0.018232379379200
F	-3.400478020127203	3.395206834624950	-0.034481225434498
F	3.393456437796922	3.395657313725778	-0.018751620114590
F	-3.399379418610074	-3.397138753055028	-0.040778585834238
F	3.392138611074464	-3.396289886495069	-0.020123912518122
H	-1.172264243295352	0.539711828456648	3.918050378595684
O	0.096703286992234	0.177629267350408	2.587262661282406
O	-1.009069519770492	-0.211381851466296	3.294939694382828

Transition Metal: Cu; Functional Group: H; Adsorbate: Clean

Cu	0.000000000000000	-0.000087667348232	0.024140526004930
C	0.685115481583826	4.253648141163142	-0.013976395651596
C	1.106054696616578	2.866019089887332	0.005265066946756
C	2.436534270681486	2.436590250562252	0.006272424124262
C	-0.685096629137956	-4.253638683357259	-0.012895862947062
C	-1.106049075125071	-2.866045692519958	0.005450111863230
C	-2.436554972076660	-2.436602168745637	0.007334014925342
C	0.685096629137958	-4.253638683357259	-0.012895862947062
C	1.106049075125074	-2.866045692519958	0.005450111863230
C	-0.685115481583821	4.253648141163142	-0.013976395651596
C	2.436554972076664	-2.436602168745637	0.007334014925342
C	-4.253460771298872	0.685117249580226	-0.001678107101270
C	-1.106054696616578	2.866019089887332	0.005265066946756
C	-2.865815806797492	1.106027936244540	0.010255535054018
C	-4.253393342920706	-0.685080576873872	-0.000957445029293
C	-2.865748806551661	-1.106069693152524	0.010986151744230
C	-2.436534270681491	2.436590250562252	0.006272424124262
C	4.253460771298876	0.685117249580226	-0.001678107101270
C	2.865815806797488	1.106027936244540	0.010255535054018
C	4.253393342920702	-0.685080576873872	-0.000957445029293
C	2.865748806551652	-1.106069693152524	0.010986151744230
N	0.000000000000000	2.035838764517584	0.016940952413748
N	0.000000000000000	-2.035848670018613	0.016054175730872
N	-2.035516953305351	0.000039130547676	0.018080535870532
N	2.035516953305352	0.000039130547676	0.018080535870532
H	5.107541822562732	-1.359844190764495	-0.009088110122228
H	-5.107551988498793	1.360084519254266	-0.010911497859297
H	-5.107541822562720	-1.359844190764495	-0.009088110122228
H	-1.359969499588509	5.107731261064387	-0.027948471752428
H	1.359969499588506	5.107731261064387	-0.027948471752428
H	5.107551988498789	1.360084519254266	-0.010911497859297
H	-1.359881768709510	-5.107764347830479	-0.025649640841142
H	1.359881768709508	-5.107764347830479	-0.025649640841142
H	-3.208799602987852	3.208749722504472	-0.002173491034390
H	3.208799602987848	3.208749722504472	-0.002173491034390
H	-3.208835480713560	-3.208703161139322	-0.000087645264692
H	3.208835480713568	-3.208703161139322	-0.000087645264692

Transition Metal: Cu; Functional Group: H; Adsorbate: O

Cu	0.000000000000000	-0.000893258760210	0.240593393716536
C	0.685361304982324	4.253791343425871	-0.015673568381153
C	1.107248480051892	2.866661701439852	0.001706497296714
C	2.437535537125748	2.434767983974182	0.001610088672424
C	-0.685249835223026	-4.254717622441856	-0.015557531641566
C	-1.107115467099579	-2.867303073633398	-0.002170535420376
C	-2.437302332632587	-2.435088188675859	0.001465204134010
C	0.685249835223030	-4.254717622441856	-0.015557531641566
C	1.107115467099580	-2.867303073633398	-0.002170535420376
C	-0.685361304982326	4.253791343425871	-0.015673568381153
C	2.437302332632590	-2.435088188675859	0.001465204134010
C	-4.260043339347664	0.684814602164854	-0.006746306937810
C	-1.107248480051890	2.866661701439852	0.001706497296714
C	-2.871330915401099	1.105345346095784	-0.009117337217734
C	-4.259897696545824	-0.685186205896407	-0.005567204135275
C	-2.871101190486854	-1.105553231524638	-0.008229085304294
C	-2.437535537125747	2.434767983974182	0.001610088672424
C	4.260043339347664	0.684814602164854	-0.006746306937810
C	2.871330915401104	1.105345346095784	-0.009117337217734
C	4.259897696545828	-0.685186205896407	-0.005567204135275
C	2.871101190486856	-1.105553231524638	-0.008229085304294
N	0.000000000000000	2.040355665844966	0.001727970477694
N	0.000000000000000	-2.041314983525123	-0.006800547236729
N	-2.045311008291534	0.000081229169276	-0.027420669138326
N	2.045311008291538	0.000081229169276	-0.027420669138326
H	5.113507525608586	-1.360699350822692	-0.004329533431555
H	-5.114025686300653	1.359872479725840	-0.006769856119369
H	-5.113507525608584	-1.360699350822692	-0.004329533431555
H	-1.359829445112346	5.108146730765966	-0.032762118669652
H	1.359829445112348	5.108146730765966	-0.032762118669652
H	5.114025686300652	1.359872479725840	-0.006769856119369
H	-1.359853798725791	-5.108900668474233	-0.028682840219815
H	1.359853798725788	-5.108900668474233	-0.028682840219815
H	-3.208711409588989	3.208101828706018	0.008775764314000
H	3.208711409588990	3.208101828706018	0.008775764314000
H	-3.208830471612124	-3.207934116995300	0.012835926784530
H	3.208830471612124	-3.207934116995300	0.012835926784530
O	0.000000000000000	-0.024168997565965	2.206615393872418

Transition Metal: Cu; Functional Group: H; Adsorbate: OH

Cu	0.000000000000000	-0.004520693721418	0.230152188184790
C	0.685584907725002	4.254189750654768	-0.014570612464389
C	1.107390567671316	2.867192569787840	-0.001253578790776
C	2.437790216442208	2.433334550189376	-0.005950750142462
C	-0.684975952539300	-4.257699001379631	-0.017450763770672
C	-1.104870885799659	-2.868496931549803	-0.013874189465910
C	-2.435318083800123	-2.435687244833066	-0.006531375493806
C	0.684975952539296	-4.257699001379631	-0.017450763770672
C	1.104870885799654	-2.868496931549803	-0.013874189465910
C	-0.685584907725001	4.254189750654768	-0.014570612464389
C	2.435318083800126	-2.435687244833066	-0.006531375493806
C	-4.260833578554738	0.683287073535530	-0.008312070719430
C	-1.107390567671310	2.867192569787840	-0.001253578790776
C	-2.871803593025675	1.103659753713992	-0.017056413584449
C	-4.260029697721087	-0.686757917418944	-0.006128740567792
C	-2.870522222691807	-1.106154120856154	-0.015304308775564
C	-2.437790216442213	2.433334550189376	-0.005950750142462
C	4.260833578554738	0.683287073535530	-0.008312070719430
C	2.871803593025674	1.103659753713992	-0.017056413584449
C	4.260029697721090	-0.686757917418944	-0.006128740567792
C	2.870522222691808	-1.106154120856154	-0.015304308775564
N	0.000000000000000	2.039528570668238	0.000295259693430
N	0.000000000000000	-2.042209316876729	-0.023508998871595
N	-2.044874275635241	-0.001049236160718	-0.037943810530773
N	2.044874275635244	-0.001049236160718	-0.037943810530773
H	5.113601855680656	-1.362466193958376	-0.000918395416288
H	-5.115000786480435	1.358191616220906	-0.004663836599683
H	-5.113601855680658	-1.362466193958376	-0.000918395416288
H	-1.360305018400634	5.108458611051761	-0.031059612514944
H	1.360305018400636	5.108458611051761	-0.031059612514944
H	5.115000786480438	1.358191616220906	-0.004663836599683
H	-1.360329723746414	-5.111491654069072	-0.022127702311607
H	1.360329723746412	-5.111491654069072	-0.022127702311607
H	-3.209387646461540	3.206130144771496	0.001672265574554
H	3.209387646461544	3.206130144771496	0.001672265574554
H	-3.206622547401654	-3.208772185656436	0.010458839728236
H	3.206622547401652	-3.208772185656436	0.010458839728236
H	0.000000000000000	0.931148312214058	2.548583020698514
O	0.000000000000000	0.001433959629178	2.246138641985796

Transition Metal: Cu; Functional Group: H; Adsorbate: OOH

Cu	0.059118595633992	0.011473440562238	0.011554276132296
C	0.732811422849978	4.261594760892144	-0.047197465710539
C	1.153256654546372	2.873397774427948	-0.043957468261100
C	2.484134070215376	2.444777949488240	-0.063014225922944
C	-0.643161214942882	-4.238739377807583	-0.009399822077700
C	-1.062466925998542	-2.850410060673735	0.008848040554998
C	-2.394341726406772	-2.425141213427260	0.039711784964446
C	0.726190242150054	-4.239776387057994	-0.035879943513478
C	1.148860254314684	-2.852182607479982	-0.036537521559512
C	-0.636499742083551	4.262679696067840	-0.019517804265657
C	2.480346696486316	-2.425982884732065	-0.056027218300146
C	-4.210158698756732	0.701104611129266	0.027499194657470
C	-1.058081156384297	2.875158820160984	0.003059186285102
C	-2.827848585086670	1.124821527790564	0.062029851629526
C	-4.211108803445365	-0.671629720520780	0.029143405702254
C	-2.829236887980088	-1.096953164642866	0.064351210793356
C	-2.390682050385248	2.452169509948356	0.035287042313958
C	4.303298043223812	0.692769833492772	-0.079177353728387
C	2.915155791213126	1.114744908660862	-0.061145070622551
C	4.302323281324668	-0.677072784839790	-0.076676224663355
C	2.913522440864202	-1.096728546948114	-0.057584132243218
N	0.047333438074462	2.043874353943600	-0.016506382680780
N	0.044253970157696	-2.021032485263440	-0.012817956678166
N	-1.993130763689830	0.013479677268698	0.111513023693500
N	2.086113384687298	0.009625488459910	-0.045450616766260
H	5.155392886907038	-1.353196336324118	-0.085970370827398
H	-5.064812633252432	1.374540212835496	-0.000567177327182
H	-5.066825477122093	-1.344054648025981	0.002670818698022
H	-1.311979833275466	5.116237438724315	-0.011265049077807
H	1.408703372249658	5.114473139872739	-0.069803263966612
H	5.157015044013894	1.368076555649398	-0.091163156890390
H	-1.319946934071016	-5.091312719097507	0.001515682807706
H	1.400679738472712	-5.093825704791703	-0.054495981690174
H	-3.158310631491201	3.228566938220252	0.025002058409468
H	3.255457652828710	3.217703552747604	-0.079489071146288
H	-3.163525206267778	-3.200193092541749	0.031339790729662
H	3.250143128850794	-3.200294754173868	-0.068960100534964
H	-1.795000311342207	0.022207307150502	2.251557700367472
O	-0.374688585442532	0.000439644541564	3.475639212457104
O	-1.709303941640052	0.020029346313420	3.248571098257802

Transition Metal: Cu; Functional Group: NH2; Adsorbate: Clean

Cu	0.018597806553024	-0.020131280520751	-0.031171634556294
C	0.871161849121270	4.158536117482342	-0.675375174792276
C	1.239429127293788	2.771080432221394	-0.485596019769797
C	2.563642767183300	2.253460043223168	-0.503114489083387
C	-0.773125793470129	-4.175455988501859	-0.566449795689504
C	-1.191605645128512	-2.825197130186986	-0.257570560454951
C	-2.524686066485582	-2.343637455999733	-0.214525071101715
C	0.589284603800948	-4.245099105126576	-0.307547042604803
C	0.994810609869460	-2.922224910406950	0.129049183659674
C	-0.487538596783097	4.253212106427488	-0.414560278344261
C	2.318963017871450	-2.548519329095210	0.476445631205998
C	-4.134820348520467	0.825165417139562	0.581073924631000
C	-0.960982469545506	2.907874634248178	-0.148804487324185
C	-2.782193203377677	1.214253321437728	0.243420150137348
C	-4.194044096371892	-0.558288186096576	0.493524476054942
C	-2.876261057098755	-1.002438930698197	0.087889373190162
C	-2.317818165904630	2.546629768799222	0.060637155598574
C	4.234454834701141	0.554947269516520	0.380558622284900
C	2.918202420230014	0.940524661573674	-0.101227257307716
C	4.146827204979118	-0.782241299327019	0.741789222247304
C	2.798986315789952	-1.214685952801755	0.441524567877098
N	0.117426430433958	2.032632283727110	-0.152109003921137
N	-0.096212059547259	-2.071240059937697	0.133307405137312
N	-2.021214188242883	0.084725494096690	-0.011029555464649
N	2.060133623068348	-0.143950251440334	-0.042596103875681
N	5.212030935422852	-1.593967596792840	1.280051764002170
N	-5.231163134938351	1.698339667285592	0.884669654412336
N	-5.337067524459666	-1.343448829637858	0.758036403972366
N	-1.241910746093538	5.446763560213093	-0.449741541675888
N	1.756238988551430	5.249083943960605	-1.013322721560826
N	5.386295131559188	1.350624357967912	0.476826144853516
N	-1.614594824141694	-5.253931758456879	-1.027326602339677
N	1.389940430062246	-5.390984643647577	-0.447020363020204
N	-3.277112843087160	3.585200088700890	0.080414538723556
N	3.629216674939244	3.130791687818646	-0.818549678625562
N	-3.578012169266323	-3.266526016146877	-0.390283641932211
N	3.232383059126476	-3.589855947625868	0.752995450725520
H	-1.397899611456729	-6.127480688757787	-0.537201628131726
H	-1.500287851031569	-5.430589600228297	-2.031715015644782
H	-3.235716535970074	-4.194463386372870	-0.670263412137174
H	-4.325639370242158	-2.931327313980660	-0.998728591123648
H	-5.214384964431375	2.047890541206694	1.848206047643204
H	-6.129228123043136	1.235744267189246	0.726446175755466
H	-1.903571005033299	5.519142051604358	0.326541667642044
H	1.409571547965556	5.785264245637628	-1.813962573138635
H	1.887827229289840	5.902369954789978	-0.232979404800066
H	3.291960791190198	4.053909572061054	-1.120321833684809
H	4.294990211420850	2.729130706866200	-1.479991136027660
H	5.175854631818382	2.351824893270944	0.471290673828740
H	5.987968834293921	1.089816013256430	1.259767116619308
H	6.096010934282871	-1.411208370146049	0.794648296209714
H	5.368171401802668	-1.412932111219774	2.278051409410058
H	4.153694002542975	-3.231428468625964	1.035466713831824
H	2.872751325625726	-4.288598552355044	1.404084752830678
H	2.384008587345230	-5.169071351009451	-0.538266545080948
H	1.071966816181908	-6.007780066119619	-1.196582238632438
H	-5.098706563429209	-2.324892695647865	0.919839752470882
H	-5.883089790273942	-0.977041157017130	1.541513403961316
H	-4.238227440088348	3.226207334724020	0.077679950430424
H	-3.128090691375981	4.281169870237808	-0.651325960267691
H	-0.637339124598157	6.271419644222902	-0.466345483173459

Transition Metal: Cu; Functional Group: NH2; Adsorbate: O

Cu	0.034576361242356	-0.141496123739572	0.667216144914808
C	0.912859619592052	4.116608832848324	-0.914622236782801
C	1.259778488844860	2.772903846754690	-0.486885408998710
C	2.574916930117094	2.285185328625312	-0.197468275663390
C	-0.854673446051855	-4.120538767992294	-0.782856982036549
C	-1.218245253118535	-2.802143460065064	-0.305037061633300
C	-2.545643439487684	-2.310754555222854	-0.071429909189209
C	0.533686661334684	-4.195486578564179	-0.725124655563111
C	0.993135672078616	-2.922808516237549	-0.208255799171420
C	-0.468482254583282	4.219013167888320	-0.790446645513235
C	2.340828031222798	-2.583980054963263	0.133926974582708
C	-4.093398968853997	0.891452257069850	0.760057777226124
C	-0.927919102770645	2.916996861438844	-0.336847904122060
C	-2.754400121181192	1.239196014089574	0.326494805271228
C	-4.168159818356473	-0.496464524273875	0.742444950528710
C	-2.878823516030700	-0.966563084062127	0.278796300359314
C	-2.284384676449719	2.563614973992818	0.019680171703342
C	4.149586154556754	0.523144010160416	0.814750844562046
C	2.893897252696180	0.952626487179020	0.236806918794646
C	4.111725056104302	-0.865779701066604	0.867754368318192
C	2.815498189296040	-1.255347586768302	0.356608336046484
N	0.120806898428130	2.062888156504148	-0.196315856158012
N	-0.085566201819987	-2.087008124461441	0.001861825004898
N	-2.020403047830829	0.102150596745258	0.091077486309394
N	2.077362089794920	-0.138106886114763	0.019312847855158
N	5.129064964411319	-1.761087946414772	1.371699233375894
N	-5.147836641413852	1.810440474144010	1.106542846810660
N	-5.303007016203566	-1.276480341740577	1.079303895465178
N	-1.287727822872007	5.383921914825064	-1.045352246634842
N	1.805896906522100	5.154453167554486	-1.304993468967016
N	5.225495604388716	1.363461128496772	1.228487109837822
N	-1.763158099936216	-5.153913206814078	-1.225141516013405
N	1.317243133510796	-5.318935618074029	-1.069365684954754
N	-3.190832918230409	3.575824076774326	0.058741751926764
N	3.623239921890976	3.165554188711802	-0.338677292829267
N	-3.576573892140630	-3.229987450277957	-0.160672743708496
N	3.265325683467028	-3.615533875996103	0.220464555947534
H	-1.549960697427682	-6.057014859388774	-0.790488184636814
H	-1.738538154743331	-5.285558476738370	-2.242525967336206
H	-3.312129304581475	-4.134531390581310	-0.569538214498223
H	-4.496993059487203	-2.869908568671171	-0.402979715063886
H	-5.154606669298358	2.037878688620984	2.107253787029116
H	-6.070722103815298	1.443999186740962	0.859918795074932
H	-0.940963428094125	6.213257054128696	-0.554073428367624
H	2.398936821830008	4.876134971802094	-2.093045540927456
H	1.292015321640272	5.995869627161106	-1.581718155555070
H	3.422618601649454	4.164325201531168	-0.333787104688419
H	4.550749525916472	2.855220247707468	-0.052448612181173
H	4.930273969938378	2.007794119005558	1.969355066610514
H	6.000281152879304	0.806666773212538	1.599485030022044
H	6.049933090157968	-1.568879166254586	0.967117189320198
H	5.217442450379184	-1.705305034862587	2.392335289793600
H	4.156916654169088	-3.338384552304891	0.650171086162396
H	2.903593890630800	-4.521608217183237	0.511956279440850
H	2.222533253246434	-5.068057042624483	-1.471331800689676
H	0.822361339331162	-5.952135744319060	-1.701035788500512
H	-5.046231723574419	-2.149653734727199	1.545735071887834
H	-5.945010695427053	-0.759829728675406	1.686272368737812
H	-4.163083644940993	3.350205982105356	0.281469808315286
H	-2.888049462181172	4.502572928558606	-0.252921482806602
H	-1.341644527056804	5.612665849475256	-2.043692590061056
O	0.204848157570526	0.362183324740970	2.392741533949152

Transition Metal: Cu; Functional Group: NH2; Adsorbate: OH

Cu	0.031481948033880	-0.025761127193334	0.486180968904806
C	0.912079064190066	4.015901495099258	-1.108298145659393
C	1.268281362046470	2.751506638372118	-0.503049812826770
C	2.578362594656658	2.293485909044772	-0.151228526898556
C	-0.841576076279438	-4.096923481351860	-0.794539169571028
C	-1.211818613324549	-2.788647182008081	-0.290401080348488
C	-2.531531597172034	-2.294646745248873	-0.047585931477869
C	0.544721428619482	-4.174208631400028	-0.704997183807961
C	0.988646904169578	-2.910842057365866	-0.144159692626494
C	-0.472907309700503	4.125219196913284	-1.005087652389474
C	2.319074494718446	-2.567477925002414	0.244845353280962
C	-4.039576897868004	0.907919322005050	0.851122685515814
C	-0.929718471473628	2.900459041896962	-0.381157112979608
C	-2.722827387507714	1.262606408364766	0.368621595760918
C	-4.109880624944983	-0.480150849236786	0.835619655680122
C	-2.840136156669722	-0.950064153146297	0.323143526211972
C	-2.276761009004471	2.577509232550962	0.019431304613032
C	4.113823541859136	0.547478252958934	0.928946816982108
C	2.879971943750040	0.975187754767392	0.302182850456238
C	4.051221477349538	-0.837015447035597	1.024614177603608
C	2.771781333828400	-1.232798281654834	0.477250551953960
N	0.129169614572678	2.081708112043760	-0.117074848317472
N	-0.090589632383779	-2.084330798914017	0.061909471566788
N	-1.990845804106058	0.121802782363886	0.102832754048208
N	2.055778874287902	-0.119654525838044	0.083821169451970
N	5.047202431327560	-1.720689684580531	1.579631310339186
N	-5.083006399786427	1.824028438353410	1.221739025931880
N	-5.227563976260070	-1.262488726349986	1.219027803752596
N	-1.307987569186466	5.228618543576315	-1.418882146672878
N	1.812650824125600	4.978090760171368	-1.662520348352864
N	5.199214888587002	1.361333688853996	1.332666663624910
N	-1.747031029608639	-5.115614348514972	-1.273617785652220
N	1.342196759827318	-5.283289972667831	-1.058895016999912
N	-3.179062158217601	3.602134672744614	0.058264699006474
N	3.606720874682164	3.218885113095620	-0.185630037880877
N	-3.574317119150503	-3.203872821347776	-0.139392938332811
N	3.251073473870932	-3.593697727736675	0.351893468222044
H	-1.512170415428923	-6.037958175115865	-0.894540354989882
H	-1.743007039886351	-5.191632821996286	-2.296849496928612
H	-3.315904901957374	-4.105131887860569	-0.557967373175899
H	-4.488037102615380	-2.835887162450618	-0.395054530179799
H	-4.992878777042296	2.151978133860734	2.189549904922450
H	-6.011914515358114	1.411306182897556	1.111022153137108
H	-0.906412529089131	6.134177016717840	-1.160967983641506
H	2.327586221984664	4.592378071793156	-2.460881651854098
H	1.303387770719598	5.798812146477498	-2.003131243092469
H	3.389084446381074	4.154068385247412	-0.525913763647090
H	4.559892581883839	2.886323549261814	-0.299626551908009
H	4.891879451168927	2.238067959996556	1.759406954723866
H	5.810297460583234	0.870712283976106	1.989844408568034
H	5.996623812964453	-1.451149241233846	1.308472951503532
H	5.007605932540255	-1.752024905705074	2.604410138967888
H	4.135102721148586	-3.307072270957864	0.789723154795692
H	2.889536476326644	-4.494423064488863	0.661153354448232
H	2.275903875016646	-5.019143286749257	-1.378167449618545
H	0.891001745359542	-5.879171209871409	-1.755984700606909
H	-4.948531729140432	-2.161104098444106	1.618936075437508
H	-5.811941831761171	-0.770644074882803	1.899751375439450
H	-4.158148386621059	3.376032361901192	0.238905754631882
H	-2.897223612833180	4.494476428090900	-0.352089693224524
H	-1.472415993858132	5.236860012661609	-2.431293912710956
H	0.088730075734376	1.107103183062318	2.669463180676634
O	0.105896402800646	0.153023396051684	2.469467322957314

Transition Metal: Cu; Functional Group: NH2; Adsorbate: OOH

Cu	-0.010998696915362	0.062450451551636	0.177436988334968
C	0.901639673880474	3.999352848437512	-1.165107877289099
C	1.260039015114916	2.741207367986044	-0.550982671254555
C	2.572783174614406	2.287591802866740	-0.224328536177282
C	-0.904187412788659	-4.008221127622368	-0.721355345505089
C	-1.296256429658044	-2.725152137982427	-0.190712310477842
C	-2.616095426864810	-2.223683288283166	-0.038366813368956
C	0.477647410613898	-4.106057279707123	-0.573340423606496
C	0.912636943108826	-2.875452350460336	0.048021679996474
C	-0.474868409332469	4.138845666545672	-1.015479703845273
C	2.241072466202104	-2.544433013883975	0.430666810787816
C	-4.077959676139075	1.002642828838822	0.844915735125162
C	-0.942349959571246	2.934052897107318	-0.368382078547913
C	-2.759989759817913	1.340175095764440	0.355447932831164
C	-4.178133190149813	-0.382602815166216	0.803246690083264
C	-2.917877835632325	-0.869253005355976	0.282611120626416
C	-2.285529050074867	2.651901807645238	0.050869327987544
C	4.096832073357186	0.569092248989780	0.898610299157650
C	2.867264419061448	0.984671815799012	0.249780991546996
C	3.999358270933252	-0.801884265140195	1.091558357699446
C	2.711172490940236	-1.207869519838447	0.574280890750570
N	0.114395413547978	2.093379540374510	-0.123610193949929
N	-0.176177131946250	-2.041062212177366	0.265192140821884
N	-2.056418580771570	0.190455964615374	0.052815817989876
N	2.021522783097120	-0.106446847484751	0.102348516606496
N	4.983038739141034	-1.666106796019886	1.690868792421124
N	-5.109325306046040	1.923423006828726	1.219867942050002
N	-5.307835123201945	-1.139265672072078	1.191614316633972
N	-1.297322253428817	5.251242772686174	-1.424906897584407
N	1.792302093663512	4.935859203102024	-1.769974260666718
N	5.196426974161690	1.374568670977666	1.253403291580420
N	-1.785316740671984	-5.000792964842971	-1.283454255059048
N	1.272168047776654	-5.201831024633698	-0.955370975047778
N	-3.153985679772809	3.711559026674432	0.160464424521036
N	3.620850558528974	3.219422375120492	-0.267637564658813
N	-3.684394421939587	-3.124117020042604	-0.155959293129566
N	3.163278603478624	-3.595830432495092	0.562260740528764
H	-1.482845471453018	-5.946528066092620	-1.032382090395284
H	-1.827392964526304	-4.951769655097840	-2.307521774555454
H	-3.396652422554276	-4.039048914256632	-0.521779128766521
H	-4.513573287351331	-2.750848142632595	-0.617348073639544
H	-4.961589408997861	2.331929604113692	2.148537779286984
H	-6.031174314187542	1.482050061156178	1.205533373904342
H	-0.878126399004614	6.152342671455449	-1.181083907563568
H	2.305858587892054	4.518854581293134	-2.552342443694389
H	1.278203466323434	5.740548920702260	-2.138606174359762
H	3.365670155367358	4.142868831678550	-0.618030623093020
H	4.513886700415625	2.877534588679446	-0.618286421128836
H	4.929054807286052	2.341464058152872	1.447942990813834
H	5.717014861838386	0.987498424958264	2.043387699742698
H	5.936102651241733	-1.369690253992829	1.464690618043914
H	4.897898935028148	-1.701207848400013	2.712715603926202
H	4.065013612958850	-3.283379218485706	0.942998266546096
H	2.799376325273660	-4.418517905520345	1.043001967842434
H	2.258834068601972	-4.959863002626548	-1.063495731945608
H	0.919089943841624	-5.678951528984623	-1.786575625836743
H	-5.067378810977258	-2.110169874647678	1.402566408222610
H	-5.785259416959709	-0.725861401575973	1.996597565603446
H	-4.147798268909899	3.493481264252040	0.242819570543040
H	-2.861054063674398	4.581014834860112	-0.290863391503336
H	-1.482217618689276	5.252490457266926	-2.433480512071032
H	-0.047430478521970	-1.743546539042386	2.166728084203664
O	0.143105717235946	0.041746232250336	2.704115476551164
O	0.229540184505758	-1.308823741715678	3.028325215252330

Transition Metal: Cu; Functional Group: OH; Adsorbate: Clean

H	9.411799999999999	16.880220000000001	8.187770000000000
H	7.980410000000000	15.239369999999999	7.228940000000000
H	12.428550000000000	5.365150000000000	6.499540000000000
H	14.036890000000000	6.761810000000000	7.502990000000000
H	10.101920000000000	4.850940000000000	7.891290000000000
H	11.973100000000001	17.135370000000002	7.459720000000000
H	6.725330000000000	7.973740000000000	8.388990000000000
H	17.123519999999999	11.991099999999999	8.333270000000001
H	16.087340000000001	8.626180000000000	7.759200000000000
H	15.261210000000000	14.058600000000000	8.416610000000000
H	5.907190000000000	13.379250000000001	7.533160000000000
H	4.861100000000000	10.026100000000000	8.169079999999999
C	10.320750000000000	15.244270000000000	7.618080000000000
C	9.907380000000000	13.869619999999999	7.659700000000000
C	8.580819999999999	13.417780000000000	7.535830000000000
C	11.666399999999999	6.784070000000000	7.611350000000000
C	12.086420000000000	8.155830000000000	7.683330000000000
C	13.419490000000000	8.600220000000000	7.620120000000000
C	10.309030000000000	6.741810000000000	7.854550000000000
C	9.884490000000000	8.117419999999999	8.008680000000000
C	11.685790000000001	15.283910000000001	7.813430000000000
C	8.552040000000000	8.559780000000000	8.159330000000001
C	15.223030000000000	11.677420000000000	8.146540000000000
C	12.108950000000000	13.909610000000001	7.981150000000000
C	13.854210000000000	12.122930000000000	8.068840000000000
C	15.234730000000001	10.318569999999999	7.934800000000000
C	13.854830000000000	9.925240000000001	7.763760000000000
C	13.439610000000000	13.468850000000000	8.153499999999999
C	6.759210000000000	11.698760000000000	7.809130000000000
C	8.143760000000000	12.093570000000000	7.687330000000000
C	6.766740000000000	10.346310000000001	8.060499999999999
C	8.138640000000001	9.904330000000000	8.045740000000000
O	9.478170000000000	16.348179999999999	7.370820000000000
O	7.570770000000000	14.346000000000000	7.294940000000000
O	12.507040000000000	5.664690000000000	7.426550000000000
O	14.436859999999999	7.660660000000000	7.461140000000000
O	9.512110000000000	5.630130000000000	7.911800000000000
O	12.490090000000000	16.393920000000001	7.830970000000000
O	7.621160000000000	7.575060000000000	8.376150000000001
O	16.302479999999999	12.515290000000000	8.380649999999999
O	16.371500000000001	9.549519999999999	7.928530000000000
O	14.365629999999999	14.456340000000001	8.379600000000000
O	5.621650000000000	12.463720000000000	7.738060000000000
O	5.681940000000000	9.510619999999999	8.277180000000000
Cu	10.998889999999999	11.012090000000001	7.868970000000000
N	11.007989999999999	13.065630000000001	7.895370000000000
N	10.986700000000001	8.960570000000001	7.921350000000000
N	13.025309999999999	11.033930000000000	7.829010000000000
N	8.973039999999999	10.990449999999999	7.814500000000000

Transition Metal: Cu; Functional Group: OH; Adsorbate: O

H	9.461850000000000	16.896930000000001	7.737400000000000
H	7.977910000000000	15.267650000000000	6.835950000000000
H	12.520080000000000	5.321120000000000	5.849760000000000
H	14.011410000000000	6.714270000000000	7.065410000000000
H	10.051930000000000	4.787630000000000	6.948860000000000
H	11.947340000000001	17.227150000000002	6.729590000000000
H	6.675450000000000	7.971400000000000	7.346580000000000
H	17.135770000000001	12.000069999999999	7.477860000000000
H	16.121559999999999	8.602160000000000	7.350920000000000
H	15.291720000000000	14.025740000000001	7.330690000000000
H	5.887230000000000	13.406879999999999	7.041720000000000
H	4.826380000000000	10.020120000000000	7.272830000000000
C	10.314230000000000	15.313630000000000	6.957270000000000
C	9.923380000000000	13.923420000000000	6.971910000000000
C	8.593109999999999	13.438190000000001	7.002350000000000
C	11.663090000000000	6.719090000000000	6.923970000000000
C	12.070300000000000	8.089060000000000	7.083010000000000
C	13.408040000000000	8.555140000000000	7.133550000000000
C	10.283200000000001	6.679300000000000	7.003940000000000
C	9.857040000000000	8.055059999999999	7.176960000000000
C	11.694200000000000	15.351240000000001	6.983670000000000
C	8.519940000000000	8.533060000000001	7.273910000000000
C	15.227819999999999	11.670420000000000	7.370420000000000
C	12.118259999999999	13.957560000000001	7.040530000000000
C	13.852919999999999	12.101680000000000	7.251810000000000
C	15.239870000000000	10.294409999999999	7.344240000000000
C	13.856030000000001	9.890530000000000	7.221900000000000
C	13.449339999999999	13.467540000000000	7.169300000000000
C	6.747160000000000	11.711630000000000	7.184050000000000
C	8.143610000000001	12.100660000000000	7.132140000000000
C	6.738710000000000	10.338690000000000	7.286370000000000
C	8.111240000000000	9.895920000000000	7.280850000000000
O	11.242620000000001	11.446149999999999	9.495300000000000
O	9.437519999999999	16.419609999999999	6.884560000000000
O	7.575740000000000	14.368860000000000	6.920990000000000
O	12.522880000000001	5.608150000000000	6.784130000000000
O	14.418290000000001	7.612880000000000	7.103090000000000
O	9.476290000000001	5.576860000000000	6.917420000000000
O	12.503159999999999	16.458010000000002	6.963980000000000
O	7.568870000000000	7.560880000000000	7.322290000000000
O	16.314340000000001	12.526140000000000	7.463810000000000
O	16.386920000000000	9.541800000000000	7.416550000000000
O	14.402490000000000	14.434630000000000	7.234090000000000
O	5.606050000000000	12.472939999999999	7.129830000000000
O	5.642250000000000	9.492419999999999	7.359670000000000
Cu	10.994920000000000	10.880940000000001	7.822140000000000
N	11.031680000000000	13.123849999999999	7.004200000000000
N	10.959420000000000	8.885520000000000	7.226520000000000
N	13.025069999999999	10.997520000000000	7.162780000000000
N	8.959660000000000	10.985820000000000	7.198860000000000

Transition Metal: Cu; Functional Group: OH; Adsorbate: OH

H	10.971360000000001	10.161590000000000	9.714589999999999
H	9.480860000000000	16.936360000000001	7.424870000000000
H	7.971460000000000	15.265230000000001	6.677930000000000
H	12.533110000000001	5.334740000000000	5.684310000000000
H	14.023410000000000	6.732520000000000	6.888730000000000
H	10.068099999999999	4.797600000000000	6.813590000000000
H	11.969560000000000	17.171759999999999	6.450350000000000
H	6.695240000000000	7.971720000000000	7.301210000000000
H	17.121710000000000	11.994579999999999	7.531610000000000
H	16.091860000000000	8.601950000000000	7.248380000000000
H	15.286199999999999	14.045100000000000	7.363080000000000
H	5.894070000000000	13.404730000000001	7.039550000000000
H	4.857120000000000	10.015760000000000	7.349640000000000
C	10.319470000000001	15.287120000000000	6.787280000000000
C	9.917270000000000	13.907790000000000	6.878690000000000
C	8.584820000000001	13.438219999999999	6.886590000000000
C	11.672310000000000	6.732480000000000	6.755270000000000
C	12.076620000000000	8.105560000000001	6.904780000000000
C	13.410019999999999	8.571380000000000	6.960640000000000
C	10.295040000000000	6.689390000000000	6.855310000000000
C	9.868460000000001	8.066090000000001	7.027040000000000
C	11.698420000000000	15.323320000000001	6.846030000000000
C	8.535259999999999	8.536260000000000	7.156150000000000
C	15.219189999999999	11.672779999999999	7.357970000000000
C	12.122520000000000	13.942850000000000	7.001080000000000
C	13.854810000000001	12.115309999999999	7.201630000000000
C	15.225440000000001	10.300100000000000	7.273950000000000
C	13.846019999999999	9.904350000000001	7.085070000000000
C	13.453419999999999	13.474930000000001	7.159290000000000
C	6.761310000000000	11.711130000000001	7.156520000000000
C	8.147069999999999	12.105070000000000	7.017320000000000
C	6.765380000000000	10.340600000000000	7.271770000000000
C	8.134950000000000	9.896890000000001	7.176470000000000
O	11.007720000000001	11.079079999999999	9.384010000000000
O	9.451079999999999	16.386630000000000	6.617210000000000
O	7.567400000000000	14.370290000000001	6.781540000000000
O	12.533810000000001	5.621950000000000	6.618480000000000
O	14.427630000000001	7.631890000000000	6.921500000000000
O	9.488939999999999	5.584700000000000	6.791920000000000
O	12.511049999999999	16.424579999999999	6.771900000000000
O	7.586570000000000	7.560990000000000	7.245990000000000
O	16.300850000000001	12.521470000000001	7.533980000000000
O	16.363170000000000	9.536420000000000	7.359660000000000
O	14.396630000000000	14.452280000000000	7.270240000000000
O	5.620650000000000	12.474110000000000	7.176110000000000
O	5.677840000000000	9.494050000000000	7.426380000000000
Cu	10.996850000000000	11.021800000000001	7.415620000000000
N	11.026190000000000	13.109980000000000	7.004920000000000
N	10.966950000000001	8.900350000000000	7.055500000000000
N	13.023870000000001	11.020410000000000	7.027310000000000
N	8.971460000000000	10.991260000000000	7.016210000000000

Transition Metal: Cu; Functional Group: OH; Adsorbate: OOH

H	9.5315100000000001	16.927640000000000	6.774650000000000
H	8.012000000000000	15.319750000000001	5.954710000000000
H	12.564170000000001	5.433470000000000	5.084120000000000
H	14.054720000000000	6.744840000000000	6.374040000000000
H	10.081890000000000	4.881190000000000	6.129610000000000
H	11.993810000000000	17.177879999999998	5.722000000000000
H	6.696610000000000	8.011590000000000	6.497010000000000
H	17.172460000000001	12.012409999999999	6.663680000000000
H	16.116510000000002	8.620660000000001	6.584920000000000
H	15.346570000000000	14.079400000000000	6.398710000000000
H	5.935350000000000	13.463419999999999	6.195370000000000
H	4.867640000000000	10.084500000000000	6.495010000000000
H	11.107130000000000	9.265820000000000	8.439510000000000
C	10.363750000000000	15.298819999999999	6.083630000000000
C	9.948140000000000	13.926570000000000	6.172690000000000
C	8.611929999999999	13.483240000000000	6.148680000000000
C	11.685250000000000	6.796600000000000	6.183190000000000
C	12.111359999999999	8.151490000000001	6.361610000000000
C	13.446389999999999	8.591210000000000	6.373250000000000
C	10.304539999999999	6.766350000000000	6.249240000000000
C	9.876540000000000	8.132099999999999	6.433490000000000
C	11.742900000000001	15.325680000000000	6.096950000000000
C	8.541740000000001	8.587550000000000	6.464580000000000
C	15.270040000000000	11.699040000000000	6.499180000000000
C	12.168460000000000	13.946600000000000	6.230970000000000
C	13.903549999999999	12.141330000000000	6.366790000000000
C	15.267780000000000	10.325030000000000	6.508560000000000
C	13.883740000000000	9.924849999999999	6.389790000000000
C	13.505920000000000	13.494930000000000	6.312800000000000
C	6.782490000000000	11.761979999999999	6.316440000000000
C	8.172050000000000	12.153490000000000	6.232060000000000
C	6.777780000000000	10.392420000000000	6.431780000000000
C	8.147330000000000	9.944080000000000	6.406640000000000
O	9.507759999999999	16.411680000000000	5.944850000000000
O	7.597940000000000	14.428879999999999	6.043530000000000
O	12.522700000000000	5.673400000000000	6.030840000000000
O	14.464200000000000	7.639330000000000	6.355140000000000
O	9.500330000000000	5.667200000000000	6.130670000000000
O	12.551360000000001	16.426570000000002	6.004210000000000
O	7.588560000000000	7.604030000000000	6.520480000000000
O	16.360440000000001	12.547960000000000	6.593090000000000
O	16.399410000000000	9.558160000000001	6.628600000000000
O	14.454269999999999	14.483300000000000	6.343940000000000
O	5.648220000000000	12.532450000000001	6.305080000000000
O	5.682670000000000	9.550750000000001	6.547820000000000
O	11.170450000000001	10.818280000000000	9.492910000000000
O	11.197780000000000	9.466960000000000	9.427099999999999
Cu	11.027790000000000	11.063079999999999	6.347640000000000
N	11.058970000000000	13.115480000000000	6.282570000000000
N	10.997100000000000	8.968230000000000	6.546750000000000
N	13.062910000000000	11.038910000000000	6.287570000000000
N	8.993850000000000	11.036880000000000	6.269390000000000

Transition Metal: Fe; Functional Group: BH2; Adsorbate: Clean

H	8.333290000000000	16.591390000000001	6.156200000000000
H	10.016909999999999	17.619190000000000	6.779770000000000
H	6.217640000000000	13.805160000000001	8.387620000000000
H	6.778770000000000	15.425400000000000	7.360230000000000
H	11.700450000000000	4.378630000000000	6.906350000000000
H	13.352270000000001	5.378100000000000	6.167510000000000
H	14.879580000000001	6.584670000000000	7.302080000000000
H	15.608770000000000	8.237700000000000	6.400020000000000
H	8.989260000000000	4.940490000000000	8.307869999999999
H	8.709780000000000	5.154550000000000	6.275920000000000
H	13.706400000000000	15.600840000000000	6.233460000000000
H	12.916600000000001	17.293630000000000	7.028060000000000
H	6.229000000000000	7.708330000000000	7.642210000000000
H	7.669580000000000	6.273730000000000	7.639390000000000
H	16.424700000000001	13.414770000000001	8.608359999999999
H	17.471450000000001	11.959080000000000	7.574020000000000
H	15.495860000000000	8.191060000000000	8.323050000000000
H	17.164459999999998	8.980610000000000	7.474570000000000
H	13.641920000000001	15.766500000000001	8.151330000000000
H	15.286429999999999	14.977430000000000	7.296230000000000
H	4.536500000000000	12.992030000000000	7.573880000000000
H	6.066620000000000	13.761229999999999	6.467430000000000
H	4.903040000000000	8.902350000000000	6.605950000000000
H	4.980680000000000	8.986820000000000	8.667669999999999
C	10.148310000000000	15.280130000000000	7.060110000000000
C	9.672020000000000	13.890020000000000	7.180340000000000
C	8.334949999999999	13.438060000000000	7.269300000000000
C	11.584840000000000	6.718230000000000	7.133520000000000
C	12.043990000000001	8.117509999999999	7.193200000000000
C	13.358060000000000	8.590330000000000	7.244600000000000
C	10.191430000000000	6.769970000000000	7.291840000000000
C	9.843740000000000	8.169729999999999	7.362700000000000
C	11.546460000000000	15.188230000000001	7.158790000000000
C	8.488740000000000	8.557869999999999	7.463680000000000
C	15.114409999999999	11.716790000000000	7.506640000000000
C	11.879560000000000	13.803000000000001	7.273340000000000
C	13.716310000000000	12.177450000000000	7.435510000000000
C	15.045100000000000	10.324040000000000	7.397480000000000
C	13.649240000000001	9.972580000000001	7.327690000000000
C	13.251899999999999	13.495210000000000	7.361170000000000
C	6.669430000000000	11.673760000000000	7.461810000000000
C	8.057359999999999	12.074180000000000	7.362790000000000
C	6.659880000000000	10.282940000000000	7.513690000000000
C	8.071960000000001	9.899680000000000	7.449340000000000
B	9.424490000000000	16.577259999999999	6.655860000000000
B	6.950640000000000	14.244120000000001	7.352130000000000
B	12.290340000000000	5.415720000000000	6.724970000000000
B	14.728199999999999	7.767800000000000	7.301120000000000
B	9.109999999999999	5.620490000000000	7.316220000000000
B	12.830100000000000	16.104659999999999	7.125730000000000
B	7.447180000000000	7.492330000000000	7.572840000000000
B	16.418839999999999	12.441000000000001	7.905270000000000
B	15.972049999999999	9.054919999999999	7.409580000000000
B	14.097870000000000	14.854530000000000	7.279070000000000
B	5.729080000000000	12.927510000000000	7.484030000000000
B	5.508330000000000	9.214079999999999	7.604490000000000
Fe	10.860340000000001	11.017289999999999	7.326330000000000
N	10.751780000000000	13.001320000000000	7.280380000000000
N	10.943410000000000	8.994130000000000	7.299340000000000
N	12.839370000000001	11.084830000000000	7.346620000000000
N	8.913840000000000	10.979540000000000	7.361970000000000

Transition Metal: Fe; Functional Group: BH2; Adsorbate: O

C	10.149340000000000	15.276870000000001	6.739260000000000
C	9.678960000000000	13.882190000000000	6.856420000000000
C	8.343230000000000	13.427149999999999	6.918180000000000
C	11.580019999999999	6.718330000000000	6.813540000000000
C	12.035629999999999	8.124210000000000	6.869370000000000
C	13.347210000000000	8.601870000000000	6.896690000000000
C	10.190980000000000	6.763260000000000	6.978680000000000
C	9.842990000000000	8.169400000000000	7.049310000000000
C	11.543770000000000	15.195650000000001	6.846550000000000
C	8.486250000000000	8.553060000000000	7.137970000000000
C	15.127929999999999	11.718769999999999	7.111860000000000
C	11.882800000000000	13.806310000000000	6.962850000000000
C	13.725160000000001	12.184979999999999	7.079350000000000
C	15.043850000000001	10.328030000000000	6.999540000000000
C	13.644240000000000	9.984590000000001	6.962670000000000
C	13.257440000000001	13.504560000000000	7.034950000000000
C	6.667710000000000	11.666470000000000	7.058450000000000
C	8.061840000000000	12.062700000000000	6.989220000000000
C	6.650740000000000	10.278269999999999	7.118180000000000
C	8.067729999999999	9.893190000000001	7.086400000000000
B	9.422860000000000	16.571770000000001	6.323060000000000
B	6.957520000000000	14.237200000000000	6.974610000000000
B	12.286370000000000	5.418270000000000	6.389890000000000
B	14.718080000000000	7.773070000000000	6.926830000000000
B	9.097110000000001	5.622940000000000	6.987230000000000
B	12.822760000000001	16.115580000000001	6.809320000000000
B	7.450650000000000	7.479500000000000	7.257730000000000
B	16.447430000000001	12.431190000000001	7.480080000000000
B	15.966469999999999	9.052420000000000	6.995480000000000
B	14.096240000000000	14.870390000000000	6.952460000000000
B	5.731050000000000	12.926320000000000	7.065910000000000
B	5.491660000000000	9.217810000000000	7.194410000000000
H	8.369669999999999	16.574100000000001	5.746780000000000
H	9.978619999999999	17.622450000000001	6.517950000000000
H	6.199030000000000	13.796939999999999	7.989100000000000
H	6.792360000000000	15.419710000000000	6.981260000000000
H	11.726350000000000	4.375370000000000	6.622070000000000
H	13.316710000000000	5.391050000000000	5.774960000000000
H	14.861020000000000	6.588480000000000	6.930560000000000
H	15.578810000000001	8.229120000000000	6.000810000000000
H	8.993900000000000	4.907120000000000	7.955390000000000
H	8.679360000000001	5.191870000000000	5.938170000000000
H	13.695090000000000	15.618399999999999	5.910790000000000
H	12.905049999999999	17.305199999999999	6.717440000000000
H	6.232450000000000	7.683000000000000	7.298140000000000
H	7.691890000000000	6.266630000000000	7.378350000000000
H	16.481510000000000	13.445660000000000	8.120699999999999
H	17.486010000000000	11.896910000000000	7.186460000000000
H	15.510820000000001	8.196380000000000	7.927340000000000
H	17.159790000000001	8.975320000000000	7.032350000000000
H	13.639580000000000	15.774410000000000	7.830860000000000
H	15.282810000000000	15.002910000000000	6.961270000000000
H	4.537320000000000	12.994730000000001	7.128280000000000
H	6.093560000000000	13.765260000000000	6.064200000000000
H	4.928640000000000	8.870220000000000	6.183600000000000
H	4.934590000000000	9.007500000000000	8.245400000000000
O	10.882750000000000	11.029230000000000	8.908040000000000
N	10.759729999999999	13.006900000000000	6.963080000000000
N	10.937160000000000	8.988670000000001	6.979660000000000
N	12.848280000000001	11.099720000000000	6.997300000000000
N	8.907579999999999	10.970850000000000	6.996720000000000
Fe	10.860690000000000	11.026230000000000	7.261040000000000

Transition Metal: Fe; Functional Group: BH2; Adsorbate: OH

C	10.146870000000000	15.286610000000000	6.637770000000000
C	9.675219999999999	13.894790000000000	6.767630000000000
C	8.336620000000000	13.433240000000000	6.816080000000000
C	11.579319999999999	6.717360000000000	6.705430000000000
C	12.036490000000001	8.122000000000000	6.774740000000000
C	13.347040000000000	8.603960000000001	6.798840000000000
C	10.188890000000001	6.762800000000000	6.869640000000000
C	9.842590000000000	8.169930000000001	6.956520000000000
C	11.544650000000001	15.205190000000000	6.734830000000000
C	8.483510000000001	8.554169999999999	7.042770000000000
C	15.131530000000000	11.725390000000001	7.003920000000000
C	11.882650000000000	13.818770000000001	6.862800000000000
C	13.728740000000000	12.192420000000000	6.975780000000000
C	15.044810000000000	10.333240000000000	6.900360000000000
C	13.644950000000000	9.989580000000000	6.871670000000000
C	13.258780000000000	13.512359999999999	6.921910000000000
C	6.663120000000000	11.669879999999999	6.938820000000000
C	8.056419999999999	12.069419999999999	6.887410000000000
C	6.649830000000000	10.281190000000000	7.006360000000000
C	8.070200000000000	9.899710000000001	6.995280000000000
B	9.420669999999999	16.580890000000000	6.217700000000000
B	6.947580000000000	14.240060000000000	6.851920000000000
B	12.285340000000000	5.416630000000000	6.282100000000000
B	14.718750000000000	7.778240000000000	6.815040000000000
B	9.092079999999999	5.625030000000000	6.872880000000000
B	12.824850000000000	16.122380000000000	6.672780000000000
B	7.446370000000000	7.487590000000000	7.144250000000000
B	16.453009999999999	12.438390000000000	7.359790000000000
B	15.967700000000001	9.056970000000000	6.888090000000000
B	14.098509999999999	14.876420000000000	6.812420000000000
B	5.723180000000000	12.927090000000000	6.931230000000000
B	5.498500000000000	9.209989999999999	7.076090000000000
H	10.934220000000000	11.807720000000000	9.578630000000000
H	8.361430000000000	16.581920000000000	5.654180000000000
H	9.982290000000001	17.631200000000000	6.396520000000000
H	6.175470000000000	13.802910000000001	7.857190000000000
H	6.780870000000000	15.422400000000000	6.853700000000000
H	11.714860000000000	4.375480000000000	6.495110000000000
H	13.326129999999999	5.386990000000000	5.685840000000000
H	14.864280000000001	6.594370000000000	6.807330000000000
H	15.577260000000001	8.243160000000000	5.888900000000000
H	8.982310000000000	4.914030000000000	7.844130000000000
H	8.689980000000000	5.185260000000000	5.821620000000000
H	13.685060000000000	15.612810000000000	5.768250000000000
H	12.907970000000001	17.310749999999999	6.565720000000000
H	6.226390000000000	7.698400000000000	7.186170000000000
H	7.679330000000000	6.269870000000000	7.241300000000000
H	16.492030000000000	13.468420000000000	7.974590000000000
H	17.488990000000001	11.890610000000001	7.082560000000000
H	15.516270000000000	8.196000000000000	7.815460000000000
H	17.160959999999999	8.979910000000000	6.921910000000000
H	13.654740000000000	15.791630000000000	7.686300000000000
H	15.284910000000000	15.006779999999999	6.805510000000000
H	4.528420000000000	12.992360000000000	6.978150000000000
H	6.096400000000000	13.766000000000000	5.931600000000000
H	4.933490000000000	8.870310000000000	6.063510000000000
H	4.931750000000000	9.008380000000001	8.124079999999999
O	10.874499999999999	10.959270000000000	9.101470000000001
N	10.754870000000000	13.022770000000000	6.890260000000000
N	10.936420000000000	8.982749999999999	6.902910000000000
N	12.852560000000000	11.105250000000000	6.913140000000000
N	8.903490000000000	10.973929999999999	6.918250000000000
Fe	10.864350000000000	11.030189999999999	7.222820000000000

Transition Metal: Fe; Functional Group: BH2; Adsorbate: OOH

C	10.136780000000000	15.265180000000001	6.444520000000000
C	9.666890000000000	13.871580000000000	6.590750000000000
C	8.330740000000000	13.412950000000000	6.674020000000000
C	11.573100000000000	6.695870000000000	6.441780000000000
C	12.028910000000000	8.098630000000000	6.548240000000000
C	13.339230000000001	8.579250000000000	6.600420000000000
C	10.180479999999999	6.738720000000000	6.588030000000000
C	9.832979999999999	8.143060000000000	6.705300000000000
C	11.534030000000000	15.181260000000000	6.519660000000000
C	8.475490000000001	8.527930000000000	6.801030000000000
C	15.117880000000000	11.702360000000001	6.822990000000000
C	11.872439999999999	13.793550000000000	6.650900000000000
C	13.717430000000000	12.168830000000000	6.779170000000000
C	15.034160000000000	10.308059999999999	6.727050000000000
C	13.636469999999999	9.963930000000000	6.684610000000000
C	13.247730000000001	13.489179999999999	6.712440000000000
C	6.661350000000000	11.648560000000000	6.803370000000000
C	8.051679999999999	12.048120000000001	6.747870000000000
C	6.647530000000000	10.256930000000001	6.833690000000000
C	8.064230000000000	9.874370000000001	6.803600000000000
B	9.403390000000000	16.556419999999999	6.031540000000000
B	6.943090000000000	14.219690000000000	6.738050000000000
B	12.286429999999999	5.408120000000000	5.995390000000000
B	14.709580000000001	7.752880000000000	6.635800000000000
B	9.086470000000000	5.600100000000000	6.550090000000000
B	12.814750000000000	16.098130000000001	6.447920000000000
B	7.434050000000000	7.462140000000000	6.867040000000000
B	16.435220000000001	12.420870000000001	7.185010000000000
B	15.957680000000000	9.032900000000000	6.726440000000000
B	14.087410000000000	14.852200000000000	6.595120000000000
B	5.720220000000000	12.905550000000000	6.822360000000000
B	5.493430000000000	9.187220000000000	6.871150000000000
H	8.321859999999999	16.556870000000000	5.511410000000000
H	9.978300000000001	17.605850000000000	6.170410000000000
H	6.186310000000000	13.770040000000000	7.750530000000000
H	6.774360000000000	15.401590000000001	6.757630000000000
H	11.708489999999999	4.361910000000000	6.158910000000000
H	13.343200000000000	5.394530000000000	5.426750000000000
H	14.854260000000000	6.568770000000000	6.635650000000000
H	15.582120000000000	8.216270000000000	5.722410000000000
H	8.961560000000000	4.865840000000000	7.501650000000000
H	8.692420000000000	5.192000000000000	5.483300000000000
H	13.672700000000001	15.582360000000000	5.546290000000000
H	12.897670000000000	17.285799999999998	6.331740000000000
H	6.214160000000000	7.675510000000000	6.919890000000000
H	7.661340000000000	6.241530000000000	6.914540000000000
H	16.466449999999998	13.451150000000000	7.799920000000000
H	17.475149999999999	11.878010000000000	6.913190000000000
H	15.492770000000000	8.172160000000000	7.647270000000000
H	17.150369999999999	8.955330000000000	6.777900000000000
H	13.645060000000001	15.775330000000000	7.463240000000000
H	15.274300000000000	14.982279999999999	6.584550000000000
H	4.526010000000000	12.968909999999999	6.888270000000000
H	6.075640000000000	13.755450000000000	5.826580000000000
H	4.921270000000000	8.891240000000000	5.848630000000000
H	4.930510000000000	8.947419999999999	7.912980000000000
H	10.391540000000001	10.292550000000000	10.546480000000001
O	10.999739999999999	10.981550000000000	8.904310000000001
O	10.033099999999999	10.193479999999999	9.638800000000000
N	10.747120000000001	12.997809999999999	6.694180000000000
N	10.927310000000000	8.958980000000000	6.679560000000000
N	12.841580000000000	11.081280000000000	6.715030000000000
N	8.900869999999999	10.951680000000000	6.753330000000000
Fe	10.856220000000000	11.001980000000000	6.972560000000000

Transition Metal: Fe; Functional Group: CH3; Adsorbate: Clean

H	9.171239999999999	16.221920000000001	9.059659999999999
H	10.610749999999999	17.135980000000000	8.598430000000000
H	9.233499999999999	17.057160000000000	7.494490000000000
H	6.617840000000000	14.209800000000000	7.267910000000000
H	7.229070000000000	14.843400000000001	8.805630000000001
H	7.862680000000000	15.436660000000000	7.260610000000000
H	12.453560000000000	5.669130000000000	9.701779999999999
H	11.945650000000001	4.796510000000000	8.247660000000000
H	13.429100000000000	5.752380000000000	8.226039999999999
H	14.777300000000000	8.763489999999999	10.050190000000001
H	13.515200000000000	7.546800000000000	10.217150000000000
H	14.804090000000000	7.319800000000000	9.023720000000001
H	9.517790000000000	5.322510000000000	6.175680000000000
H	10.040699999999999	4.742450000000000	7.764500000000000
H	8.556100000000001	5.683900000000000	7.618810000000000
H	12.268039999999999	17.240259999999999	7.474970000000000
H	13.664220000000000	16.163850000000000	7.299420000000000
H	12.757450000000000	16.691929999999999	5.870910000000000
H	8.472410000000000	7.091860000000000	5.280260000000000
H	7.181360000000000	7.050640000000000	6.492310000000000
H	7.197960000000000	8.307869999999999	5.244120000000000
H	16.405560000000001	13.357360000000000	6.883760000000000
H	17.294799999999999	11.834530000000001	6.914620000000000
H	16.481929999999998	12.350009999999999	5.428840000000000
H	16.618030000000001	9.659070000000000	9.155310000000000
H	16.252070000000000	8.543440000000000	7.829220000000000
H	17.250520000000002	9.967850000000000	7.531250000000000
H	14.907810000000000	14.746540000000000	5.980320000000000
H	14.672250000000000	13.470850000000000	4.774550000000000
H	13.502950000000000	14.782810000000000	4.900610000000000
H	4.871800000000000	11.535800000000000	8.690189999999999
H	5.818550000000000	12.965220000000000	9.112040000000000
H	4.998540000000000	12.871869999999999	7.540990000000000
H	5.789530000000000	8.420349999999999	7.669360000000000
H	4.739110000000000	9.846670000000000	7.655970000000000
H	5.325770000000000	9.174759999999999	6.134540000000000
C	10.451689999999999	15.231320000000000	7.606470000000000
C	9.942460000000001	13.860530000000001	7.612850000000000
C	8.591469999999999	13.454549999999999	7.760920000000000
C	11.602430000000000	6.924760000000000	8.128010000000000
C	11.994930000000000	8.331410000000000	8.152550000000000
C	13.269130000000001	8.840990000000000	8.505369999999999
C	10.379130000000000	6.856000000000000	7.476140000000000
C	9.975680000000001	8.228669999999999	7.193890000000000
C	11.731159999999999	15.188350000000000	7.074220000000000
C	8.701420000000001	8.653879999999999	6.753340000000000
C	15.151289999999999	11.585580000000000	6.986220000000000
C	12.052700000000000	13.783970000000000	6.870370000000000
C	13.760910000000001	12.009000000000000	6.861070000000000
C	15.145440000000001	10.409390000000000	7.723460000000000
C	13.748230000000000	10.060800000000000	7.961850000000000
C	13.303369999999999	13.275630000000000	6.433250000000000
C	6.790400000000000	11.611010000000000	7.714230000000000
C	8.167350000000001	12.103630000000001	7.675990000000000
C	6.813310000000000	10.299450000000000	7.265820000000000
C	8.212859999999999	9.946360000000000	7.074850000000000
C	9.827249999999999	16.465720000000001	8.213800000000001
C	7.522550000000000	14.540160000000000	7.786050000000000
C	12.395460000000000	5.733260000000000	8.602430000000000
C	14.141810000000000	8.070840000000000	9.484750000000000
C	9.586169999999999	5.594730000000000	7.242160000000000
C	12.652040000000000	16.371910000000000	6.921500000000000
C	7.837880000000000	7.722070000000000	5.916200000000000
C	16.387660000000000	12.316420000000001	6.526730000000000
C	16.371390000000002	9.607170000000000	8.081569999999999
C	14.147550000000001	14.118230000000001	5.489110000000000

C	5.566160000000000	12.287269999999999	8.286250000000001
C	5.615290000000000	9.389010000000001	7.176790000000000
Fe	10.971080000000001	11.050530000000000	7.414680000000000
N	10.981859999999999	12.995550000000000	7.267360000000000
N	10.982519999999999	9.099320000000001	7.593820000000000
N	12.931469999999999	11.044879999999999	7.426320000000000
N	9.016830000000001	11.036170000000000	7.381520000000000

Transition Metal: Fe; Functional Group: CH3; Adsorbate: O

H	9.260560000000000	16.156970000000001	9.152450000000000
H	10.687300000000000	17.076440000000002	8.666029999999999
H	9.270460000000000	17.037150000000000	7.610810000000000
H	6.630710000000000	14.208760000000000	7.404130000000000
H	7.305300000000000	14.776479999999999	8.940860000000001
H	7.878830000000000	15.431929999999999	7.397540000000000
H	12.365670000000000	5.748270000000000	9.785420000000000
H	11.900210000000000	4.829810000000000	8.345850000000000
H	13.388970000000000	5.776240000000000	8.339470000000000
H	14.702489999999999	8.843830000000001	10.084450000000000
H	13.436410000000000	7.631760000000000	10.252370000000001
H	14.755010000000000	7.372900000000000	9.098430000000000
H	9.522240000000000	5.331080000000000	6.162900000000000
H	10.017690000000000	4.758570000000000	7.764130000000000
H	8.538489999999999	5.705500000000000	7.587790000000000
H	12.278750000000000	17.221650000000000	7.431810000000000
H	13.674500000000000	16.145700000000001	7.241490000000000
H	12.745450000000000	16.663370000000000	5.823820000000000
H	8.495820000000000	7.108540000000000	5.189170000000000
H	7.191710000000000	7.064520000000000	6.389680000000000
H	7.222320000000000	8.327120000000001	5.144700000000000
H	16.391089999999998	13.373279999999999	6.864010000000000
H	17.290019999999998	11.855309999999999	6.918730000000000
H	16.481660000000002	12.348640000000000	5.421850000000000
H	16.557099999999998	9.748329999999999	9.245730000000000
H	16.250979999999998	8.590840000000000	7.939500000000000
H	17.242159999999998	10.018689999999999	7.636730000000000
H	14.891900000000000	14.725880000000000	5.875060000000000
H	14.650290000000000	13.439299999999999	4.679980000000000
H	13.480990000000000	14.753520000000000	4.800340000000000
H	4.923680000000000	11.479189999999999	8.764450000000000
H	5.878950000000000	12.896509999999999	9.204230000000001
H	5.016870000000000	12.850199999999999	7.653570000000000
H	5.797590000000000	8.411470000000000	7.621610000000000
H	4.749790000000000	9.841010000000001	7.622880000000000
H	5.345580000000000	9.189290000000000	6.095030000000000
C	10.480520000000000	15.203040000000000	7.625230000000000
C	9.964580000000000	13.834339999999999	7.609470000000000
C	8.617839999999999	13.430000000000000	7.789600000000000
C	11.571930000000000	6.952780000000000	8.143620000000000
C	11.970039999999999	8.360320000000000	8.130430000000000
C	13.234740000000000	8.878430000000000	8.501910000000001
C	10.367380000000001	6.869260000000000	7.459790000000000
C	9.977359999999999	8.235849999999999	7.129760000000000
C	11.739810000000000	15.167350000000001	7.045420000000000
C	8.710010000000000	8.661700000000000	6.667870000000000
C	15.146010000000000	11.596399999999999	6.973520000000000
C	12.048930000000000	13.766760000000000	6.801100000000000
C	13.755620000000000	12.003610000000000	6.799080000000000
C	15.128470000000000	10.440849999999999	7.741860000000000
C	13.724330000000000	10.085140000000001	7.941020000000000
C	13.293290000000001	13.259219999999999	6.344310000000000
C	6.813840000000000	11.589140000000000	7.738740000000000
C	8.189900000000000	12.083520000000000	7.676940000000000
C	6.827090000000000	10.293390000000000	7.245780000000000
C	8.221819999999999	9.947229999999999	7.014390000000000
C	9.886150000000001	16.422400000000000	8.290609999999999
C	7.556000000000000	14.515850000000000	7.898510000000000
C	12.344170000000000	5.775660000000000	8.683310000000001
C	14.081980000000000	8.135429999999999	9.522660000000000
C	9.574370000000000	5.608550000000000	7.228630000000000
C	12.656580000000000	16.351189999999999	6.877760000000000
C	7.854050000000000	7.736440000000000	5.820240000000000
C	16.382829999999998	12.327680000000001	6.519310000000000
C	16.348440000000000	9.662490000000000	8.166110000000000
C	14.129730000000000	14.094460000000000	5.390420000000000

C	5.605110000000000	12.244520000000000	8.364950000000000
C	5.627530000000000	9.387729999999999	7.142200000000000
Fe	10.970280000000001	11.025340000000000	7.041090000000000
O	10.995880000000000	10.873070000000000	5.396860000000000
N	10.990660000000000	12.979110000000000	7.215150000000000
N	10.969609999999999	9.108750000000001	7.531600000000000
N	12.923400000000001	11.055080000000000	7.365370000000000
N	9.027030000000000	11.024600000000000	7.337240000000000

Transition Metal: Fe; Functional Group: CH3; Adsorbate: OH

H	10.357730000000000	11.353389999999999	4.604840000000000
H	9.244090000000000	16.154060000000001	9.151009999999999
H	10.678870000000000	17.079809999999998	8.699540000000001
H	9.279180000000000	17.050750000000001	7.619470000000000
H	6.632230000000000	14.219970000000000	7.350560000000000
H	7.294220000000000	14.806039999999999	8.886120000000000
H	7.881090000000000	15.444310000000000	7.341190000000000
H	12.361780000000000	5.752120000000000	9.783820000000000
H	11.906980000000001	4.831650000000000	8.342060000000000
H	13.393120000000000	5.783530000000000	8.343890000000000
H	14.691780000000000	8.852119999999999	10.090949999999999
H	13.427190000000000	7.638630000000000	10.250280000000000
H	14.754860000000001	7.380080000000000	9.105470000000000
H	9.504980000000000	5.342720000000000	6.160660000000000
H	10.035209999999999	4.755940000000000	7.745980000000000
H	8.547120000000000	5.695810000000000	7.608230000000000
H	12.316900000000000	17.221209999999999	7.533120000000000
H	13.703049999999999	16.138259999999999	7.318930000000000
H	12.788850000000000	16.708510000000000	5.911590000000000
H	8.467570000000000	7.110270000000000	5.194790000000000
H	7.197480000000000	7.045600000000000	6.429960000000000
H	7.178100000000000	8.312150000000001	5.189860000000000
H	16.416180000000001	13.383360000000000	6.930810000000000
H	17.306349999999998	11.859220000000001	6.957870000000000
H	16.507220000000000	12.388920000000001	5.468040000000000
H	16.556870000000000	9.755080000000000	9.267609999999999
H	16.253940000000000	8.596069999999999	7.962320000000000
H	17.250630000000001	10.020780000000000	7.661130000000000
H	14.940020000000001	14.739210000000000	5.946420000000000
H	14.686199999999999	13.487000000000000	4.717320000000000
H	13.536160000000001	14.814439999999999	4.865610000000000
H	4.947090000000000	11.499409999999999	8.803310000000000
H	5.906590000000000	12.925970000000000	9.203010000000001
H	5.017100000000000	12.853830000000000	7.669200000000000
H	5.825930000000000	8.407500000000001	7.681450000000000
H	4.767290000000000	9.829070000000000	7.710290000000000
H	5.319320000000000	9.175300000000000	6.166600000000000
C	10.489680000000000	15.217300000000000	7.634570000000000
C	9.968420000000000	13.851430000000001	7.586610000000000
C	8.618560000000000	13.446910000000001	7.757180000000000
C	11.574149999999999	6.954770000000000	8.139060000000001
C	11.973020000000000	8.362579999999999	8.118840000000001
C	13.236850000000000	8.882830000000000	8.496480000000000
C	10.368050000000000	6.870050000000000	7.456750000000000
C	9.979770000000000	8.236549999999999	7.120670000000000
C	11.761609999999999	15.184559999999999	7.080200000000000
C	8.705320000000000	8.660560000000000	6.672050000000000
C	15.161890000000000	11.610849999999999	6.998040000000000
C	12.065780000000000	13.787530000000000	6.811510000000000
C	13.772610000000000	12.016560000000000	6.808880000000000
C	15.137340000000000	10.448610000000000	7.757520000000000
C	13.731700000000000	10.090470000000000	7.938300000000000
C	13.317930000000000	13.282270000000000	6.369320000000000
C	6.819110000000000	11.598810000000000	7.741740000000000
C	8.191030000000000	12.098120000000000	7.648400000000000
C	6.828490000000000	10.294330000000000	7.267010000000000
C	8.219049999999999	9.952349999999999	7.007920000000000
C	9.884490000000000	16.429559999999999	8.303150000000000
C	7.554190000000000	14.532880000000000	7.849320000000000
C	12.346399999999999	5.779000000000000	8.681520000000001
C	14.077109999999999	8.142280000000000	9.524380000000001
C	9.576530000000000	5.608370000000000	7.227980000000000
C	12.689850000000000	16.364570000000001	6.954780000000000
C	7.835950000000000	7.728280000000000	5.845940000000000
C	16.403919999999999	12.345100000000000	6.564160000000000
C	16.353510000000000	9.667800000000000	8.187020000000000

C	14.171180000000000	14.130820000000000	5.442600000000000
C	5.619440000000000	12.259890000000000	8.379170000000000
C	5.632440000000000	9.380080000000000	7.203740000000000
Fe	10.980840000000001	11.029660000000000	6.979380000000000
O	11.036420000000000	10.843310000000001	5.083430000000000
N	10.991370000000000	13.001550000000000	7.180600000000000
N	10.979770000000000	9.105200000000000	7.508080000000000
N	12.938879999999999	11.056670000000000	7.350470000000000
N	9.022340000000000	11.042020000000001	7.289900000000000

Transition Metal: Fe; Functional Group: CH3; Adsorbate: OOH

H	9.240610000000000	16.166740000000001	9.322070000000000
H	10.667579999999999	17.086480000000002	8.835860000000000
H	9.250430000000000	17.047249999999998	7.780540000000000
H	6.610330000000000	14.218730000000001	7.573560000000000
H	7.285080000000000	14.786740000000000	9.110820000000000
H	7.858700000000000	15.442270000000001	7.567050000000000
H	12.345720000000000	5.758330000000000	9.955290000000000
H	11.880269999999999	4.839620000000000	8.515689999999999
H	13.369220000000000	5.786160000000000	8.509250000000000
H	14.682570000000000	8.853669999999999	10.254479999999999
H	13.416539999999999	7.641620000000000	10.422340000000000
H	14.735450000000000	7.382380000000000	9.268079999999999
H	9.502319999999999	5.341190000000000	6.332900000000000
H	9.997809999999999	4.768660000000000	7.933890000000000
H	8.518700000000001	5.715500000000000	7.757470000000000
H	12.258910000000000	17.231349999999999	7.601550000000000
H	13.654529999999999	16.155539999999998	7.411290000000000
H	12.725790000000000	16.673580000000001	5.993680000000000
H	8.475849999999999	7.118450000000000	5.358780000000000
H	7.171710000000000	7.074130000000000	6.559830000000000
H	7.202700000000000	8.337040000000000	5.314480000000000
H	16.371110000000002	13.383160000000000	7.033790000000000
H	17.269839999999999	11.865209999999999	7.088440000000000
H	16.461749999999999	12.358520000000000	5.591750000000000
H	16.536890000000000	9.758310000000000	9.415520000000001
H	16.230930000000001	8.600660000000000	8.109340000000000
H	17.222380000000001	10.028570000000000	7.806490000000000
H	14.872210000000001	14.736060000000000	6.044680000000000
H	14.630730000000000	13.449249999999999	4.849420000000000
H	13.461440000000000	14.764080000000000	4.970050000000000
H	4.903620000000000	11.488920000000000	8.934279999999999
H	5.859190000000000	12.906540000000000	9.374060000000000
H	4.996760000000000	12.860250000000001	7.823150000000000
H	5.777950000000000	8.421590000000000	7.791360000000000
H	4.730150000000000	9.850830000000000	7.792670000000000
H	5.325850000000000	9.199260000000001	6.265040000000000
H	10.140409999999999	12.407800000000000	4.607620000000000
C	10.458370000000000	15.211919999999999	7.796330000000000
C	9.948910000000000	13.844670000000001	7.782700000000000
C	8.595599999999999	13.440510000000000	7.961050000000000
C	11.553699999999999	6.962230000000000	8.314530000000000
C	11.943920000000000	8.370770000000000	8.300509999999999
C	13.215470000000000	8.887460000000001	8.673489999999999
C	10.346460000000000	6.879410000000000	7.629280000000000
C	9.961790000000001	8.248279999999999	7.301610000000000
C	11.722370000000000	15.176810000000000	7.214450000000000
C	8.685359999999999	8.670870000000001	6.837100000000000
C	15.125040000000000	11.608169999999999	7.142220000000000
C	12.032019999999999	13.780189999999999	6.971770000000000
C	13.735900000000001	12.009919999999999	6.970400000000000
C	15.107550000000000	10.448079999999999	7.913460000000000
C	13.705460000000000	10.099830000000001	8.110910000000001
C	13.273569999999999	13.273490000000001	6.513970000000000
C	6.794310000000000	11.600580000000001	7.909730000000000
C	8.171790000000000	12.089380000000000	7.849430000000000
C	6.808030000000000	10.300829999999999	7.415220000000000
C	8.201850000000000	9.956840000000000	7.186600000000000
C	9.866160000000001	16.432530000000000	8.460070000000000
C	7.536150000000000	14.525440000000000	8.068080000000000
C	12.324149999999999	5.785160000000000	8.852570000000000
C	14.061780000000001	8.145700000000000	9.692040000000000
C	9.554449999999999	5.618390000000000	7.398290000000000
C	12.636810000000001	16.361300000000000	7.047250000000000
C	7.834380000000000	7.747210000000000	5.990300000000000
C	16.362860000000001	12.337580000000001	6.688900000000000
C	16.328830000000000	9.672450000000000	8.335380000000001

C	14.109629999999999	14.103490000000001	5.560980000000000
C	5.585100000000000	12.254339999999999	8.534310000000000
C	5.607150000000000	9.397629999999999	7.311530000000000
Fe	10.943510000000000	11.047010000000000	7.317920000000000
O	10.960250000000000	10.871549999999999	5.315580000000000
O	9.905120000000000	11.450939999999999	4.584180000000000
N	10.962350000000001	13.001130000000000	7.382360000000000
N	10.957050000000001	9.102919999999999	7.703680000000000
N	12.915240000000001	11.057560000000000	7.534690000000000
N	8.996670000000000	11.038180000000001	7.508600000000000

Transition Metal: Fe; Functional Group: F; Adsorbate: Clean

Fe	0.000000000000000	0.000123109959374	-0.002580019433444
C	0.683679872212610	4.245252960770506	-0.002919082940330
C	1.106408910573854	2.865685245995752	-0.007423271112500
C	2.427301220483156	2.431656206555730	-0.005762473317678
C	-0.683639759064313	-4.245157425062649	-0.004568330433163
C	-1.106315494413138	-2.865615925830586	0.002206723095160
C	-2.427178517882314	-2.431553313174732	0.005109200301412
C	0.683639759064314	-4.245157425062649	-0.004568330433163
C	1.106315494413136	-2.865615925830586	0.002206723095160
C	-0.683679872212611	4.245252960770506	-0.002919082940330
C	2.427178517882312	-2.431553313174732	0.005109200301412
C	-4.238043240889402	0.686029936247918	-0.002644344626411
C	-1.106408910573855	2.865685245995752	-0.007423271112500
C	-2.864212150937202	1.107938392223490	-0.006090915915344
C	-4.237939382984933	-0.686158533725099	0.007992382694462
C	-2.864044709777488	-1.107795411114086	0.008657446451440
C	-2.427301220483159	2.431656206555730	-0.005762473317678
C	4.238043240889412	0.686029936247918	-0.002644344626411
C	2.864212150937202	1.107938392223490	-0.006090915915344
C	4.237939382984928	-0.686158533725099	0.007992382694462
C	2.864044709777496	-1.107795411114086	0.008657446451440
N	0.000000000000000	2.015627804930148	-0.016294814291534
N	0.000000000000000	-2.015453963299624	0.010796789265168
N	-2.015964192187056	0.000133941556010	0.000216945817922
N	2.015964192187052	0.000133941556010	0.000216945817922
F	5.325900237851070	-1.476051919859852	0.009821522132824
F	-5.326345609666719	1.475409227581650	-0.004133486489607
F	-5.325900237851073	-1.476051919859852	0.009821522132824
F	-1.478820758462906	5.330023154003401	0.000531053817172
F	1.478820758462910	5.330023154003401	0.000531053817172
F	5.326345609666716	1.475409227581650	-0.004133486489607
F	-1.478708432690162	-5.329877384430793	-0.009659583770613
F	1.478708432690162	-5.329877384430793	-0.009659583770613
F	-3.392548980949080	3.394147059149508	-0.002376414926622
F	3.392548980949078	3.394147059149508	-0.002376414926622
F	-3.392541455978524	-3.394004686680990	0.001926651451522
F	3.392541455978520	-3.394004686680990	0.001926651451522

Transition Metal: Fe; Functional Group: F; Adsorbate: O

Fe	0.000000000000000	-0.000495238659330	0.265568089457172
C	0.684301425874002	4.240521114793318	-0.001263342698074
C	1.105147726439574	2.861669438200620	-0.005865209385704
C	2.427061475598056	2.425760744112824	0.006394797450222
C	-0.684265857977255	-4.242379264669061	-0.002225424685591
C	-1.105151487577231	-2.863530581255290	-0.004755825334322
C	-2.427098929294576	-2.427764937694324	0.005339225803256
C	0.684265857977254	-4.242379264669061	-0.002225424685591
C	1.105151487577234	-2.863530581255290	-0.004755825334322
C	-0.684301425874001	4.240521114793318	-0.001263342698074
C	2.427098929294574	-2.427764937694324	0.005339225803256
C	-4.242613416133596	0.683329199903514	0.007107937348008
C	-1.105147726439576	2.861669438200620	-0.005865209385704
C	-2.863689958089822	1.104036035777222	-0.000228757201366
C	-4.242584986150529	-0.685313162573173	0.006673216697974
C	-2.863632232449852	-1.106042875442178	-0.000799162315348
C	-2.427061475598059	2.425760744112824	0.006394797450222
C	4.242613416133584	0.683329199903514	0.007107937348008
C	2.863689958089824	1.104036035777222	-0.000228757201366
C	4.242584986150524	-0.685313162573173	0.006673216697974
C	2.863632232449850	-1.106042875442178	-0.000799162315348
N	0.000000000000000	2.017099996527564	-0.026460252350950
N	0.000000000000000	-2.018868425210453	-0.023530291351220
N	-2.019153377099329	-0.000966196760556	-0.021665521582220
N	2.019153377099336	-0.000966196760556	-0.021665521582220
F	5.326104551078362	-1.480181129930234	-0.000201322892458
F	-5.326195320026947	1.478135569448382	0.000344664316656
F	-5.326104551078366	-1.480181129930234	-0.000201322892458
F	-1.479043055321029	5.324071023321548	-0.006678661137954
F	1.479043055321030	5.324071023321548	-0.006678661137954
F	5.326195320026956	1.478135569448382	0.000344664316656
F	-1.479076284196964	-5.325913296219635	-0.010123375244685
F	1.479076284196960	-5.325913296219635	-0.010123375244685
F	-3.388680897700219	3.387960500748560	0.026218590497046
F	3.388680897700212	3.387960500748560	0.026218590497046
F	-3.388707950634842	-3.390048748492521	0.021614524398200
F	3.388707950634844	-3.390048748492521	0.021614524398200
O	0.000000000000000	0.001956800804408	1.913519746177104

Transition Metal: Fe; Functional Group: F; Adsorbate: OH

Fe	0.000000000000000	0.003354935115352	0.506038461627240
C	0.687255522885386	4.274584085543906	-0.043624645079084
C	1.114623649422558	2.897320978571020	-0.022169470916624
C	2.439984023549196	2.439001715179438	-0.025908631471926
C	-0.687043190938695	-4.269572954294986	-0.032398533080624
C	-1.112512092417937	-2.890897733971848	-0.017930745695958
C	-2.438568757969868	-2.432452547150966	-0.016792936825862
C	0.687043190938704	-4.269572954294986	-0.032398533080624
C	1.112512092417940	-2.890897733971848	-0.017930745695958
C	-0.687255522885387	4.274584085543906	-0.043624645079084
C	2.438568757969868	-2.432452547150966	-0.016792936825862
C	-4.281277702272003	0.689261128009534	-0.040515037844660
C	-1.114623649422562	2.897320978571020	-0.022169470916624
C	-2.901381615331982	1.114822625291122	-0.030448631867220
C	-4.280683367845901	-0.683879389009931	-0.037102936906340
C	-2.900509755390939	-1.108727213568987	-0.025193104182442
C	-2.439984023549211	2.439001715179438	-0.025908631471926
C	4.281277702272000	0.689261128009534	-0.040515037844660
C	2.901381615331978	1.114822625291122	-0.030448631867220
C	4.280683367845912	-0.683879389009931	-0.037102936906340
C	2.900509755390932	-1.108727213568987	-0.025193104182442
N	0.000000000000000	2.068397874047196	-0.002730127839384
N	0.000000000000000	-2.063361739146661	-0.009127085809504
N	-2.073847385340898	0.003788609856964	-0.023431409919525
N	2.073847385340890	0.003788609856964	-0.023431409919525
F	5.369848264430490	-1.472486101909880	-0.045442557335886
F	-5.370767512332943	1.477706515839476	-0.051451121655066
F	-5.369848264430480	-1.472486101909880	-0.045442557335886
F	-1.472678582343715	5.365940793685800	-0.059722815879198
F	1.472678582343710	5.365940793685800	-0.059722815879198
F	5.370767512332933	1.477706515839476	-0.051451121655066
F	-1.473747402544664	-5.359871691643567	-0.045486585431564
F	1.473747402544670	-5.359871691643567	-0.045486585431564
F	-3.402809729462152	3.404968756278160	-0.031329110941492
F	3.402809729462162	3.404968756278160	-0.031329110941492
F	-3.400389803738587	-3.398458471011850	-0.013264211672274
F	3.400389803738590	-3.398458471011850	-0.013264211672274
H	0.000000000000000	0.789609978521700	2.893398853444820
O	0.000000000000000	-0.022979259924000	2.356474871987204

Transition Metal: Fe; Functional Group: F; Adsorbate: OOH

Fe	-0.005548248880286	0.000376434452414	0.241396781265668
C	0.685118475501456	4.252736871507196	-0.007568192765902
C	1.106634368479508	2.873823568214862	-0.007970323539900
C	2.428649123056952	2.436756750883114	-0.001870443289504
C	-0.688400402888316	-4.236583769719061	0.003622960444594
C	-1.111080414547502	-2.859184466549703	0.001828839134496
C	-2.433076800332042	-2.422362024760560	0.005169515457096
C	0.680597458406788	-4.234070113502176	0.007177332271860
C	1.101164632225522	-2.854707762802885	0.012366460512320
C	-0.683173711690010	4.250584233939098	-0.004191195588130
C	2.423636523628382	-2.416386137852768	0.023314906971878
C	-4.243316752139192	0.689432313400200	-0.002695355644221
C	-1.102658994569509	2.870184449370782	0.001647056109826
C	-2.862260562418168	1.108395065196354	0.005191112896214
C	-4.246806774860012	-0.678633967371688	-0.006610316112102
C	-2.868787170830899	-1.100962353037144	-0.003831748397733
C	-2.424057706580921	2.430641634261960	0.013713389184454
C	4.244116401209838	0.692691117946994	-0.007434468994703
C	2.864920019174600	1.114561916726234	-0.003643665909480
C	4.242661619841844	-0.675321368085079	-0.000207643722991
C	2.862622961145638	-1.095422156926645	0.010999118862584
N	0.002719040401652	2.025821275910640	-0.012788178563436
N	-0.006121714902636	-2.010677839849592	-0.002525440042534
N	-2.019196772643276	0.001863519082980	-0.006620223717448
N	2.016835664045270	0.009927812208086	-0.002369701166318
F	5.326460168184458	-1.471225528125132	-0.010853925191949
F	-5.326024212913937	1.486141768895168	-0.014119207377757
F	-5.332844581176255	-1.471954329391703	-0.023398315271660
F	-1.478560286783942	5.334552665306882	-0.010725738143306
F	1.478640408289090	5.338842083932724	-0.018552519066522
F	5.329622438913924	1.486589797808192	-0.029279995225618
F	-1.480649162529630	-5.323538852378515	-0.008959789676229
F	1.476114345508456	-5.318114640184262	-0.001095553774564
F	-3.387322068965432	3.392762655647598	0.022661964092740
F	3.391875579376968	3.399318765959850	0.003453038512188
F	-3.395241208048347	-3.385784136110473	0.014152378445312
F	3.385636459138420	-3.381090629713274	0.035351500621022
H	-0.277090459905413	-1.419486604134043	3.151014230084360
O	0.081499500922084	0.073283780217126	2.006994624440590
O	-0.887987062936098	-0.761220204088591	2.752529232214606

Transition Metal: Fe; Functional Group: H; Adsorbate: Clean

Fe	0.000000000000000	0.000022421415038	0.001808977764758
C	0.687701865551834	4.224170729938630	-0.008510001029087
C	1.106042782843436	2.848222181367638	-0.004667796625029
C	2.438423332854996	2.429032411139042	-0.001625269225524
C	-0.687700415068576	-4.224109784079978	-0.005582579908765
C	-1.106036603177717	-2.848186379090599	-0.001444186968751
C	-2.438414158787886	-2.429009150551007	0.000833598610912
C	0.687700415068578	-4.224109784079978	-0.005582579908765
C	1.106036603177716	-2.848186379090599	-0.001444186968751
C	-0.687701865551841	4.224170729938630	-0.008510001029087
C	2.438414158787886	-2.429009150551007	0.000833598610912
C	-4.241216858626583	0.682641403462676	0.004699336975040
C	-1.106042782843438	2.848222181367638	-0.004667796625029
C	-2.852857082536847	1.103600628009912	0.002157327076390
C	-4.241268455716860	-0.682696812478376	0.005300979810266
C	-2.852884489019353	-1.103602399693827	0.003290786131044
C	-2.438423332854999	2.429032411139042	-0.001625269225524
C	4.241216858626442	0.682641403462676	0.004699336975040
C	2.852857082536850	1.103600628009912	0.002157327076390
C	4.241268455716858	-0.682696812478376	0.005300979810266
C	2.852884489019352	-1.103602399693827	0.003290786131044
N	0.000000000000000	2.001430202648554	-0.002836913452640
N	0.000000000000000	-2.001369763964618	0.000836729954386
N	-2.002920328973378	-0.000008201004700	0.002240828092868
N	2.002920328973382	-0.000008201004700	0.002240828092868
H	5.091633705013198	-1.362427131744109	0.006273129022024
H	-5.091458621043889	1.362467603201598	0.005559286134628
H	-5.091633705013203	-1.362427131744109	0.006273129022024
H	-1.365641718727485	5.075908052656520	-0.010460390036201
H	1.365641718727484	5.075908052656520	-0.010460390036201
H	5.091458621043891	1.362467603201598	0.005559286134628
H	-1.365561209112556	-5.075907135198197	-0.008289105489663
H	1.365561209112556	-5.075907135198197	-0.008289105489663
H	-3.209376905001658	3.202224822814866	-0.003040905934011
H	3.209376905001660	3.202224822814866	-0.003040905934011
H	-3.209414002470574	-3.202152268799527	0.000205566230288
H	3.209414002470572	-3.202152268799527	0.000205566230288

Transition Metal: Fe; Functional Group: H; Adsorbate: O

Fe	0.000000000000000	-0.000911366045912	0.288871584182434
C	0.684406648063414	4.230570172806570	-0.015708175650577
C	1.102465042109496	2.846216486921408	0.006953808294748
C	2.430724969462494	2.429645803203446	0.014911644928896
C	-0.684358284129651	-4.232462240477874	-0.016326101658436
C	-1.102511327980636	-2.848151678738297	0.004881258409054
C	-2.430820904855327	-2.431543876554286	0.014682393924810
C	0.684358284129652	-4.232462240477874	-0.016326101658436
C	1.102511327980638	-2.848151678738297	0.004881258409054
C	-0.684406648063419	4.230570172806570	-0.015708175650577
C	2.430820904855326	-2.431543876554286	0.014682393924810
C	-4.231897638020394	0.683636174863102	-0.003259128967482
C	-1.102465042109490	2.846216486921408	0.006953808294748
C	-2.847466595373415	1.101477999274600	0.012525849289668
C	-4.232014489232196	-0.685037600118218	-0.002616518271619
C	-2.847577125141534	-1.103286781897960	0.012906764422388
C	-2.430724969462496	2.429645803203446	0.014911644928896
C	4.231897638020386	0.683636174863102	-0.003259128967482
C	2.847466595373412	1.101477999274600	0.012525849289668
C	4.232014489232188	-0.685037600118218	-0.002616518271619
C	2.847577125141532	-1.103286781897960	0.012906764422388
N	0.000000000000000	2.004426908109340	0.007344979248982
N	0.000000000000000	-2.006321820911129	0.004267956067052
N	-2.005706575485039	-0.000885768115582	0.009780559242666
N	2.005706575485042	-0.000885768115582	0.009780559242666
H	5.081729021588184	-1.364650464758267	-0.017631817480869
H	-5.081187243058388	1.363769250072476	-0.019455238236404
H	-5.081729021588185	-1.364650464758267	-0.017631817480869
H	-1.364351961014879	5.079951060425206	-0.034962234179588
H	1.364351961014878	5.079951060425206	-0.034962234179588
H	5.081187243058394	1.363769250072476	-0.019455238236404
H	-1.364060627651646	-5.082011661588473	-0.032875701413371
H	1.364060627651652	-5.082011661588473	-0.032875701413371
H	-3.202349270287282	3.201567330286906	0.015226125457988
H	3.202349270287276	3.201567330286906	0.015226125457988
H	-3.202467899609466	-3.203439584066704	0.016596883493660
H	3.202467899609466	-3.203439584066704	0.016596883493660
O	0.000000000000000	-0.001542964228268	1.937124737289918

Transition Metal: Fe; Functional Group: H; Adsorbate: OH

Fe	0.000000000000000	0.001399324505126	0.326340058654484
C	0.685640339273152	4.238600160028914	-0.005664785047288
C	1.105211880752088	2.855908428387056	0.019967831746386
C	2.435279770209408	2.436161134454228	-0.000733894780640
C	-0.685129307897551	-4.231947643191333	0.007035703701612
C	-1.103589855642635	-2.847742135040331	0.021163910002354
C	-2.434126088246614	-2.429469543934736	0.006389651228648
C	0.685129307897550	-4.231947643191333	0.007035703701612
C	1.103589855642638	-2.847742135040331	0.021163910002354
C	-0.685640339273153	4.238600160028914	-0.005664785047288
C	2.434126088246612	-2.429469543934736	0.006389651228648
C	-4.239340971958436	0.687349442152554	-0.062595250731814
C	-1.105211880752087	2.855908428387056	0.019967831746386
C	-2.854301417516137	1.106065882849840	-0.017190020457363
C	-4.238980781444335	-0.682082142030922	-0.058886158352948
C	-2.853980502986463	-1.100196955780280	-0.012426795086881
C	-2.435279770209402	2.436161134454228	-0.000733894780640
C	4.239340971958428	0.687349442152554	-0.062595250731814
C	2.854301417516132	1.106065882849840	-0.017190020457363
C	4.238980781444329	-0.682082142030922	-0.058886158352948
C	2.853980502986468	-1.100196955780280	-0.012426795086881
N	0.000000000000000	2.017712207556874	0.042551422046156
N	0.000000000000000	-2.011099074855697	0.030285831131300
N	-2.017961008089003	0.003244512260662	0.007095959106962
N	2.017961008088858	0.003244512260662	0.007095959106962
H	5.089501337015908	-1.360686890751118	-0.087492375743189
H	-5.089845748708131	1.365721005676806	-0.094495080698422
H	-5.089501337015914	-1.360686890751118	-0.087492375743189
H	-1.363347006509578	5.090052125964318	-0.029389210551812
H	1.363347006509586	5.090052125964318	-0.029389210551812
H	5.089845748708130	1.365721005676806	-0.094495080698422
H	-1.363256721255318	-5.083181702863111	-0.006197142293942
H	1.363256721255330	-5.083181702863111	-0.006197142293942
H	-3.206548859986519	3.208349786805902	-0.022608626628256
H	3.206548859986512	3.208349786805902	-0.022608626628256
H	-3.205058722784408	-3.202366950689139	-0.005083889860802
H	3.205058722784408	-3.202366950689139	-0.005083889860802
H	0.000000000000000	0.810028397974902	2.682085326066084
O	0.000000000000000	-0.048477883779372	2.220587710996204

Transition Metal: Fe; Functional Group: H; Adsorbate: OOH

Fe	-0.036684414143259	0.066844509718350	0.268892852546744
C	0.663384621010036	4.295593148517736	-0.124679496464246
C	1.080236816660712	2.910543180083192	-0.084534745199804
C	2.407432660771766	2.489150968373642	-0.101379702814292
C	-0.721322542038816	-4.169743276457920	0.040571328418448
C	-1.139161540260041	-2.786227714844390	0.019826955220530
C	-2.465396285392835	-2.365613350425683	-0.038141592989558
C	0.645899097641916	-4.168824974038348	0.127984880468940
C	1.064548018552062	-2.784518291587862	0.149265696481680
C	-0.703951694027030	4.297586439457506	-0.062377463480917
C	2.393294027390642	-2.365156933971075	0.192087956276898
C	-4.255885153928700	0.754644726496858	-0.021310028658206
C	-1.122714355449659	2.914162387638314	0.006020168161668
C	-2.870458156794598	1.168191638170816	0.027840280749088
C	-4.260878724920245	-0.613344199814801	-0.066797543539469
C	-2.878358951541347	-1.036146080482393	-0.034721697651742
C	-2.450598330239611	2.496653562827146	0.046473907833128
C	4.205021609076534	0.738576250045084	-0.026290587095568
C	2.821261220697402	1.160503539181040	-0.037984318212822
C	4.200853291513632	-0.626344672351259	0.077168642195262
C	2.814837396458926	-1.039506031310296	0.118812811617912
N	-0.022251503263785	2.069732957378982	-0.013992935290664
N	-0.037322598032500	-1.941496869170070	0.080583004209498
N	-2.031157804462904	0.063467039655236	0.013116337213088
N	1.974450001828708	0.062892758376230	0.040183072577916
H	5.050367597045600	-1.305637940136897	0.116622979812576
H	-5.104084580450159	1.436645558442466	-0.029641520272538
H	-5.112954105772037	-1.288262639755107	-0.119388669353789
H	-1.382017486754435	5.149209519091436	-0.069779872732340
H	1.340769903126104	5.144709832887572	-0.193826446270112
H	5.057670345354833	1.411704188599628	-0.090921322538204
H	-1.397649694888457	-5.020878467062424	-0.011844588151662
H	1.322971001701462	-5.020733543681889	0.162029011604158
H	-3.222367842497363	3.268952792305844	0.058722279551150
H	3.181227632237926	3.257350644652656	-0.155629751673492
H	-3.238915165944661	-3.135086303391880	-0.078959575630740
H	3.163585572824896	-3.136786513314778	0.249753833920528
H	-0.284878683970319	-1.415750629307293	3.025670733787766
O	0.038641994562734	0.194485250805286	2.028759795142026
O	-0.884443193683374	-0.666122461601091	2.818505330230162

Transition Metal: Fe; Functional Group: NH2; Adsorbate: Clean

Fe	0.037635785257942	-0.027279931783827	-0.059641823144897
C	0.815170826750764	4.124508493085449	-0.580478350385636
C	1.191040852233744	2.731588655623154	-0.527166041616809
C	2.513848446162756	2.234993107128700	-0.648107649144482
C	-0.716721316414272	-4.185223525346796	-0.469627674357369
C	-1.120772528395161	-2.801297740500509	-0.402052574732878
C	-2.421754154242681	-2.311536954519610	-0.587393659315406
C	0.629949231816270	-4.233162631925119	-0.144986808846269
C	1.032285700613476	-2.879745068399345	0.162627100522786
C	-0.493354905625857	4.207900540665082	-0.128229105415720
C	2.318696108398508	-2.492504538830030	0.596054499925808
C	-4.125217043070082	0.723790430557958	0.478066766822142
C	-0.954867724708627	2.854579961485228	0.083147233908446
C	-2.750624220134878	1.148234527038422	0.352040154247714
C	-4.170238220205968	-0.619932145381664	0.130436244561002
C	-2.818933965090611	-1.013696177168658	-0.178093611527238
C	-2.293045421855698	2.489400693711590	0.361195524918716
C	4.222874357423674	0.579970124973512	0.215349669229744
C	2.887368964775450	0.949680605578428	-0.209908363151865
C	4.144176519339184	-0.720069682708417	0.695269212762040
C	2.784245989835198	-1.165055713060681	0.493818145860452
N	0.102547615734004	1.964480936180748	-0.125224121064132
N	-0.037522304753971	-2.004565952651681	-0.016599137904294
N	-1.950842225835490	0.0540816663210886	0.022869439577200
N	2.012968103322104	-0.114510701384333	-0.008189274996880
N	5.233758549654200	-1.497097527175978	1.231605587334402
N	-5.249210060974747	1.543446455626594	0.834650868770416
N	-5.333665934128881	-1.419853268655181	0.100242815683628
N	-1.226628224337418	5.406837847145788	0.027632926977164
N	1.665058163317774	5.228875751644014	-0.957287777293590
N	5.381438450844734	1.363390858543774	0.171842356877468
N	-1.508998215652703	-5.316261681687070	-0.803847582404401
N	1.401809096030630	-5.420598851085455	-0.117729056394364
N	-3.232619790911311	3.519314153747586	0.594422435403032
N	3.553457549250666	3.109190838615770	-1.068207170594729
N	-3.425668830848444	-3.180055789537711	-1.112144373569418
N	3.206755553041426	-3.527818662936276	1.014420141356936
H	-2.438077186235013	-5.275303870886267	-0.377217438824907
H	-1.053232429251366	-6.173310357062148	-0.478042255636154
H	-3.027208094654267	-3.884793588501619	-1.735094237106750
H	-4.140768739001162	-2.660761315674542	-1.624220904457086
H	-5.405214964800669	1.593698265538300	1.846640406967698
H	-6.111918380884580	1.219451729722130	0.391816988269416
H	-1.747660197443366	5.438109356738206	0.906948167275986
H	1.217912577114976	5.829595369673268	-1.655238589151946
H	1.922392697894642	5.817064544292040	-0.156952843570579
H	3.184862952321212	4.030657309829330	-1.333204563656032
H	4.121976198497325	2.705866537366188	-1.814711064445287
H	5.178559871681752	2.362704168912062	0.078939406470832
H	6.034427008840616	1.162660026711194	0.930349464717682
H	6.090064686061726	-1.360493679783261	0.685684078041558
H	5.445963411644426	-1.245484326517278	2.203338292943700
H	4.137967837581932	-3.147616569251557	1.225054753235024
H	2.843805931293614	-4.040697510493338	1.821283089992578
H	2.394493723368720	-5.197227305714904	0.007797740645212
H	1.282294368438672	-5.967018412214076	-0.974561718427346
H	-5.139445717919035	-2.412942616667998	0.243019625495206
H	-6.031907248825650	-1.104483904330735	0.777048288196264
H	-4.196511975667264	3.165558098538316	0.567954018913822
H	-3.111209155993599	4.315249472767366	-0.034208793836537
H	-0.615709809799142	6.224614994165182	-0.033054096871120

Transition Metal: Fe; Functional Group: NH2; Adsorbate: O

Fe	0.026516689656266	-0.021950064657748	0.297058859094156
C	0.796028746143272	4.108040867188020	-0.576015943465237
C	1.172455185949162	2.715607073869362	-0.504573726172257
C	2.493678918246482	2.218041908084852	-0.644790852012914
C	-0.705966611349918	-4.168983805835488	-0.487417686705285
C	-1.106493772367834	-2.783084473935254	-0.416529181786927
C	-2.403761087749835	-2.291549639524078	-0.634853618327540
C	0.628564194183968	-4.224374713208576	-0.124944340296913
C	1.024758150724908	-2.870449433800406	0.206135087125764
C	-0.502036952342571	4.196719828635982	-0.095340557702180
C	2.310592504667448	-2.486734011671917	0.649414849703828
C	-4.134406020278332	0.715490068972940	0.453739059953110
C	-0.956429379461483	2.846778079170388	0.147016569671248
C	-2.757719682442328	1.141678788462106	0.366401567862736
C	-4.173939571297822	-0.616786463089817	0.066344777205720
C	-2.814276544786317	-1.000396702369994	-0.222769549209985
C	-2.297121906615690	2.480248032687272	0.432881735131904
C	4.219735526514718	0.573750386512642	0.209328389499592
C	2.876085626627756	0.936317118744760	-0.202774974656297
C	4.146860670990492	-0.721583444552497	0.701363899799306
C	2.785475810903468	-1.166603228634330	0.517562041595174
N	0.089517409961824	1.958236377804552	-0.078194904980418
N	-0.031248998570998	-1.997549020127522	0.001356950649610
N	-1.956806285394585	0.066911566957386	0.002586327890854
N	2.011735356382266	-0.130306417848164	0.006016939725388
N	5.235804814846904	-1.498225984953176	1.237409941779812
N	-5.260926272634357	1.529159991697258	0.809127889823096
N	-5.336978326422287	-1.414870616652408	-0.013081518535702
N	-1.247018851058858	5.394733091953712	0.050248537813654
N	1.638250255651962	5.203446683834397	-0.993595879669474
N	5.377476892085716	1.359255809345392	0.143861174751808
N	-1.502793461516276	-5.285461896846414	-0.876357020618123
N	1.410668035021782	-5.404630195006106	-0.112656891999872
N	-3.225825982824727	3.491884200066116	0.706821699478494
N	3.521110461826564	3.086364413368242	-1.089083137250437
N	-3.390609374821018	-3.151918592999763	-1.187832773794455
N	3.183560922722440	-3.515450356304854	1.089671324637444
H	-2.398747888637793	-5.298862942599991	-0.379844541442250
H	-1.018384909331406	-6.155868003107143	-0.640100103328475
H	-2.982958605123976	-3.899637487324263	-1.752232381482031
H	-4.078450405230086	-2.640219650847623	-1.741882117178360
H	-5.415178120552071	1.575785728631520	1.821597927430100
H	-6.122349993777066	1.203626395170446	0.365170222398484
H	-1.611270195860044	5.513733835827161	0.999679459541228
H	1.213877861199792	5.747568334871698	-1.750047468240105
H	1.851632684150382	5.847558935737424	-0.224526791856348
H	3.155985363893370	4.008371404065116	-1.356395299443641
H	4.101809385124050	2.672645079873596	-1.819576076134847
H	5.170757641963990	2.358360677772800	0.063576164660676
H	6.038416956993924	1.160782291417808	0.896220317130686
H	6.089939922552410	-1.373859518272084	0.685435360007218
H	5.452849022997311	-1.236697836278712	2.205425986949084
H	4.115089514402094	-3.144566854983182	1.313043196280092
H	2.799085682799238	-4.043938253142734	1.875250037563094
H	2.398232031834084	-5.180199937338623	0.045247872264364
H	1.321018528369358	-5.927692651109592	-0.987635448490838
H	-5.140165043396397	-2.410960161721121	0.103522625518372
H	-6.042286174591482	-1.123944118002544	0.667541438384782
H	-4.197034444955500	3.168168013643682	0.631279969421376
H	-3.052083717432939	4.359493815258110	0.196972116732626
H	-0.674949803190781	6.210845329267732	-0.180760549525388
O	0.020905755507584	0.035304900605438	1.956772538181056

Transition Metal: Fe; Functional Group: NH2; Adsorbate: OH

Fe	-0.027572624520637	-0.005780982971594	0.640483458908750
C	0.808743832738696	4.153572539951019	-0.533892968029846
C	1.183526110961266	2.761940587978338	-0.395230964341884
C	2.510141694809458	2.237149334267418	-0.482252025010922
C	-0.696172127400576	-4.146738761215564	-0.647982977905180
C	-1.1452142220538076	-2.794233718090414	-0.390724494285077
C	-2.468936482978179	-2.294529698994936	-0.536903652111665
C	0.614315295543924	-4.236241283263487	-0.187904241192051
C	0.970806996467100	-2.914536727692870	0.296265751008814
C	-0.516329452616386	4.257731964726529	-0.123128300626970
C	2.274668645254948	-2.517670512495044	0.713002366215230
C	-4.218834000473759	0.785597512292248	0.371482805933826
C	-0.979891722348516	2.914859108697244	0.150616028828166
C	-2.832032068746987	1.191930695820606	0.316068285720230
C	-4.258295167726533	-0.568505753314529	0.051758059969700
C	-2.888640836981310	-0.979792672814423	-0.181399078077888
C	-2.340077945454404	2.534514013266274	0.376735579225222
C	4.241364497603954	0.537195086857056	0.312179511995400
C	2.894737985462180	0.934495105657388	-0.068764056775880
C	4.158090337674533	-0.776545785794386	0.764593817467320
C	2.782217950874086	-1.192670529316835	0.598471242896076
N	0.081677696228476	2.034316286313552	0.015444479518542
N	-0.105254339748267	-2.064053883550166	0.156191815100302
N	-2.042631707269493	0.095675032913692	0.024466838684686
N	2.028654934515146	-0.126520143670927	0.133722596465348
N	5.248195700562880	-1.584260344797698	1.259253844899976
N	-5.356711353291956	1.624461748797052	0.635194602026774
N	-5.426133473300965	-1.349764222091967	-0.028363068172695
N	-1.273617412684743	5.459827238239648	-0.063033617496360
N	1.661863127930758	5.238075084367688	-0.962840455681555
N	5.414596857900699	1.297464067511706	0.235480154782412
N	-1.465844004206613	-5.209865698315422	-1.250188701085808
N	1.413279459591168	-5.387447325653355	-0.211744162718048
N	-3.273779233462271	3.547895869479892	0.596057951044368
N	3.555549278989900	3.113468888130300	-0.866905334339656
N	-3.472833316897635	-3.191839601168482	-0.958537296825043
N	3.162486646401790	-3.551622873032340	1.087589007110716
H	-1.385024015622786	-6.078556627244165	-0.712121427193686
H	-1.156729144897767	-5.412936383100886	-2.207412714508891
H	-3.089164810006448	-4.107173470073679	-1.227545792937214
H	-4.103110497383874	-2.808471729997748	-1.663305968627430
H	-5.596799175133352	1.662907471551252	1.631834519679542
H	-6.183104169890285	1.304970487034472	0.122760462167060
H	-1.600256788655400	5.661952390751390	0.886871046368566
H	1.325029052366430	5.669319495800074	-1.829049753779827
H	1.737235294433950	5.976457899079964	-0.255155227392109
H	3.201833672542132	4.041923531726338	-1.128951914002446
H	4.165870998715072	2.720293052469186	-1.584558739785734
H	5.237708681969783	2.305036773899144	0.242220358797034
H	6.121442101970725	1.021846355969250	0.918756358024536
H	6.056772265673104	-1.548476186989433	0.629894851972814
H	5.567082048479122	-1.272640798951358	2.183342239909776
H	4.088901882583978	-3.191101240411953	1.348152034451630
H	2.777663181634720	-4.182289313134719	1.791658325678732
H	2.412203536437102	-5.174793663446868	-0.149526566239138
H	1.199743188496592	-6.010651643917857	-0.992023489308323
H	-5.232774146673078	-2.347920282612499	0.084020506303214
H	-6.146040395389171	-1.042447815978925	0.629232945121274
H	-4.246433044842002	3.238811251900106	0.483668352877344
H	-3.056550751826205	4.430776999925234	0.131373123793322
H	-0.718894944402116	6.258473402738010	-0.383105698694614
H	0.625782618324000	0.580538043179774	2.948963544969200
O	-0.078244056887851	0.062408167960706	2.520098180109648

Transition Metal: Fe; Functional Group: NH2; Adsorbate: OOH

Fe	-0.010061627695158	-0.000025759879748	0.305965854417862
C	0.802295690418288	4.102439574598738	-0.579474705442784
C	1.175316131099110	2.709882395161182	-0.475928397290225
C	2.492027707102474	2.198481981842688	-0.601498844582505
C	-0.681586182442175	-4.098468920228761	-0.684557911827767
C	-1.121794289078885	-2.734977167030934	-0.494306685524645
C	-2.433759832973912	-2.245631507276006	-0.669187201665075
C	0.596362077472550	-4.192182720029558	-0.149392622947349
C	0.954336982696578	-2.861690172560706	0.302417532555860
C	-0.485145879779427	4.209077744775596	-0.072740238332237
C	2.236170941027914	-2.482776129410365	0.774943904777908
C	-4.135006747443237	0.756346684327942	0.484290109265268
C	-0.940778303832932	2.868319579422506	0.212604743914222
C	-2.756017942825309	1.173564075917962	0.400722780905760
C	-4.189697076025334	-0.565793353617604	0.063303284931410
C	-2.832884258787846	-0.955598083190807	-0.242230238458411
C	-2.281176893919397	2.504512385374054	0.517226314002046
C	4.193457061561544	0.542147534461168	0.289682595375988
C	2.858608175902710	0.917998472896200	-0.136168312275707
C	4.096568955735850	-0.740549452232514	0.811021897065512
C	2.729336210008056	-1.169247645655783	0.629344694058872
N	0.093882800950182	1.969591300080350	-0.011497754324260
N	-0.089768440419768	-1.981311128936312	0.061604470027748
N	-1.966533857304206	0.103545259351702	-0.001808287109536
N	1.974249225451602	-0.129094338610869	0.092030231289198
N	5.168303370941744	-1.520914137312349	1.378523671928748
N	-5.255412403592480	1.570749225537056	0.858853173718074
N	-5.360303053241928	-1.344045305304839	-0.030657803608626
N	-1.230738962261409	5.411381002770642	0.061361133257376
N	1.643247314725864	5.181351021378991	-1.041049845480096
N	5.366831395138306	1.303091110333196	0.204446215207096
N	-1.443499393200234	-5.166524291230925	-1.285913338275581
N	1.375205190351742	-5.354250363463455	-0.076623088117525
N	-3.192633000099036	3.508621621020506	0.852569153881612
N	3.531246056454462	3.052201744140580	-1.045525052617108
N	-3.438737414187607	-3.115589816962672	-1.149759012564971
N	3.103621348950300	-3.512977767440152	1.215565132666334
H	-1.422141237771029	-6.011659777852344	-0.706445032360364
H	-1.079920442121310	-5.421580860298718	-2.210826620008934
H	-3.058071917469036	-4.029479941309352	-1.424263825080494
H	-4.021972794430258	-2.700882946017817	-1.876994056925852
H	-5.407377294998410	1.590987511582676	1.873092971385216
H	-6.117032897561316	1.243331423427744	0.414788422013774
H	-1.479918197604860	5.602937216941078	1.036531314476918
H	1.268145520543712	5.626146531130244	-1.884131275946071
H	1.763664943625968	5.909751281026764	-0.329630456329227
H	3.177840556561686	3.977890919381384	-1.314839485604438
H	4.112163067666774	2.631496355910610	-1.771420599552258
H	5.179809198547513	2.305340106843550	0.116491701252538
H	6.031176236426285	1.099014534176064	0.952478880166408
H	6.021505060457521	-1.448783756692151	0.815235501012710
H	5.401566992486360	-1.213770152751582	2.329248954838512
H	4.025895192862170	-3.144518435871557	1.478994170935864
H	2.699739337062282	-4.094915986708955	1.950418561617178
H	2.372856829288578	-5.152261756704796	0.031758459988762
H	1.192593514508518	-6.010743338364490	-0.836693719022367
H	-5.151529803814219	-2.345603376394720	-0.054029377322774
H	-6.024519159949975	-1.132122622435233	0.717111032848994
H	-4.169689956668623	3.206033515439818	0.763757456260306
H	-3.002467019311492	4.405690353000654	0.403356363378344
H	-0.699276266573186	6.211311423794939	-0.291705939553665
H	-0.437819806759340	-1.620537013277580	2.755921670450274
O	-0.003541489112582	0.145118230313194	2.073644139025718
O	-0.914107698904814	-0.770475737085114	2.868417255958738

Transition Metal: Fe; Functional Group: OH; Adsorbate: Clean

H	9.382330000000000	16.827490000000001	8.182000000000000
H	7.991910000000000	15.223860000000000	7.123940000000000
H	12.400990000000000	5.378370000000000	6.477260000000000
H	14.031590000000000	6.776360000000000	7.406540000000000
H	10.126500000000000	4.887490000000000	7.991960000000000
H	11.967129999999999	17.113880000000002	7.544520000000000
H	6.749880000000000	7.988320000000000	8.489570000000001
H	17.096109999999999	11.978149999999999	8.352090000000000
H	16.068660000000001	8.637079999999999	7.673580000000000
H	15.237670000000000	14.044779999999999	8.525470000000000
H	5.927500000000000	13.363920000000000	7.433300000000000
H	4.888310000000000	10.033210000000000	8.141260000000001
C	10.325630000000000	15.217000000000001	7.596410000000000
C	9.913230000000000	13.845599999999999	7.605770000000000
C	8.589060000000000	13.410010000000000	7.476350000000000
C	11.661320000000000	6.813920000000000	7.580520000000000
C	12.080370000000000	8.184060000000001	7.610270000000000
C	13.412280000000001	8.611230000000001	7.551970000000000
C	10.318930000000000	6.775510000000000	7.890830000000000
C	9.894769999999999	8.150150000000000	8.024550000000000
C	11.682820000000000	15.253439999999999	7.834820000000000
C	8.568450000000000	8.577980000000000	8.216390000000001
C	15.195869999999999	11.667149999999999	8.186669999999999
C	12.104120000000000	13.881430000000000	7.991630000000000
C	13.828510000000000	12.110720000000001	8.138890000000000
C	15.211530000000000	10.318000000000000	7.919970000000000
C	13.836570000000000	9.925760000000000	7.756210000000000
C	13.424670000000001	13.454549999999999	8.216600000000000
C	6.783190000000000	11.698020000000000	7.777420000000000
C	8.161930000000000	12.096060000000000	7.678460000000000
C	6.792730000000000	10.353640000000000	8.068809999999999
C	8.162480000000000	9.917240000000000	8.096270000000001
Fe	10.997629999999999	11.016500000000001	7.878380000000000
O	9.490209999999999	16.326239999999999	7.350120000000000
O	7.581350000000000	14.332020000000000	7.194230000000000
O	12.497320000000000	5.690740000000000	7.398120000000000
O	14.429560000000000	7.675470000000000	7.358040000000000
O	9.533130000000000	5.663620000000000	8.023230000000000
O	12.481840000000000	16.364180000000001	7.902260000000000
O	7.645690000000000	7.591910000000000	8.466220000000000
O	16.274830000000001	12.497330000000000	8.437989999999999
O	16.352200000000000	9.557280000000000	7.862170000000000
O	14.343750000000000	14.442710000000000	8.471579999999999
O	5.642340000000000	12.450799999999999	7.650270000000000
O	5.706990000000000	9.521520000000001	8.280419999999999
N	11.010470000000000	13.020730000000000	7.844260000000000
N	10.984159999999999	9.009560000000000	7.849790000000000
N	12.987000000000000	11.024920000000000	7.890080000000000
N	9.010439999999999	11.005020000000000	7.874350000000000

Transition Metal: Fe; Functional Group: OH; Adsorbate: O

H	9.389089999999999	16.828990000000001	7.415530000000000
H	8.015280000000001	15.198829999999999	6.364530000000000
H	12.356050000000000	5.418440000000000	5.700110000000000
H	14.009460000000001	6.795790000000000	6.625250000000000
H	10.113320000000000	4.892490000000000	7.271290000000000
H	11.990480000000000	17.102470000000000	6.864030000000000
H	6.772430000000000	8.006169999999999	7.946640000000000
H	17.097159999999999	11.986129999999999	7.639460000000000
H	16.060040000000001	8.652460000000000	6.878800000000000
H	15.215999999999999	14.030300000000000	7.962970000000000
H	5.941370000000000	13.340310000000001	6.647120000000000
H	4.893550000000000	10.025790000000001	7.486940000000000
C	10.333090000000000	15.201689999999999	6.882830000000000
C	9.928400000000000	13.826440000000000	6.874920000000000
C	8.606750000000000	13.386039999999999	6.722050000000000
C	11.650130000000001	6.827820000000000	6.859510000000000
C	12.066750000000001	8.200020000000000	6.889050000000000
C	13.398020000000001	8.629189999999999	6.807070000000000
C	10.317920000000001	6.782050000000000	7.209520000000000
C	9.898440000000001	8.155700000000000	7.367900000000000
C	11.679169999999999	15.246499999999999	7.175230000000000
C	8.578600000000000	8.585699999999999	7.598570000000000
C	15.196260000000001	11.669879999999999	7.475780000000000
C	12.098810000000000	13.874100000000000	7.339680000000000
C	13.827940000000000	12.110510000000000	7.450850000000000
C	15.207929999999999	10.328430000000001	7.173160000000000
C	13.827980000000000	9.941890000000001	7.013030000000000
C	13.416380000000000	13.446389999999999	7.588420000000000
C	6.791610000000000	11.683199999999999	7.044480000000000
C	8.175030000000000	12.073850000000000	6.930030000000000
C	6.797990000000000	10.352880000000001	7.393210000000000
C	8.168170000000000	9.918720000000000	7.429310000000000
Fe	10.998500000000000	11.014189999999999	7.465700000000000
O	10.991090000000000	11.026579999999999	9.121219999999999
O	9.497430000000000	16.300450000000001	6.600690000000000
O	7.606580000000000	14.304349999999999	6.424760000000000
O	12.482350000000000	5.713340000000000	6.623350000000000
O	14.407870000000001	7.696250000000000	6.593670000000000
O	9.528470000000000	5.672750000000000	7.337400000000000
O	12.476730000000000	16.356660000000002	7.266490000000000
O	7.669860000000000	7.612670000000000	7.915580000000000
O	16.274039999999999	12.502739999999999	7.722620000000000
O	16.345980000000001	9.571000000000000	7.070840000000000
O	14.319610000000001	14.423670000000000	7.908790000000000
O	5.654550000000000	12.431250000000000	6.877330000000000
O	5.716250000000000	9.522169999999999	7.630970000000000
N	11.022449999999999	13.013230000000000	7.135970000000000
N	10.975910000000001	9.014950000000001	7.158070000000000
N	12.987150000000000	11.038370000000000	7.164780000000000
N	9.013859999999999	10.986510000000001	7.144450000000000

Transition Metal: Fe; Functional Group: OH; Adsorbate: OH

H	11.116730000000000	10.211860000000000	9.777520000000001
H	9.414370000000000	16.857460000000000	7.309820000000000
H	8.000150000000000	15.207150000000000	6.340740000000000
H	12.377100000000000	5.433440000000000	5.546720000000000
H	14.019750000000000	6.781710000000000	6.561700000000000
H	10.088690000000000	4.868920000000000	6.997580000000000
H	11.994719999999999	17.103130000000000	6.670110000000000
H	6.738420000000000	7.973280000000000	7.697530000000000
H	17.104379999999999	11.988220000000000	7.471620000000000
H	16.060730000000000	8.642690000000000	6.824040000000000
H	15.240750000000000	14.045220000000000	7.758690000000000
H	5.937940000000000	13.347810000000001	6.608680000000000
H	4.882790000000000	10.011440000000000	7.293570000000000
C	10.332590000000000	15.212719999999999	6.787160000000000
C	9.922079999999999	13.841020000000000	6.825120000000000
C	8.597390000000001	13.394959999999999	6.696360000000000
C	11.648280000000000	6.809070000000000	6.732440000000000
C	12.071000000000000	8.174840000000000	6.830000000000000
C	13.402559999999999	8.611840000000001	6.767310000000000
C	10.300770000000000	6.758810000000000	7.029120000000000
C	9.884100000000000	8.126020000000000	7.234890000000000
C	11.689870000000001	15.256340000000000	7.034880000000000
C	8.559650000000000	8.559350000000000	7.437760000000000
C	15.199960000000001	11.670780000000001	7.371480000000000
C	12.106019999999999	13.886860000000000	7.226020000000000
C	13.831899999999999	12.112439999999999	7.353800000000000
C	15.208119999999999	10.321009999999999	7.103810000000000
C	13.827460000000000	9.928680000000000	6.967800000000000
C	13.427809999999999	13.455450000000001	7.454270000000000
C	6.786140000000000	11.681839999999999	6.968910000000000
C	8.170040000000000	12.077380000000000	6.883990000000000
C	6.788580000000000	10.338979999999999	7.269010000000000
C	8.158140000000000	9.902250000000000	7.310950000000000
Fe	10.994380000000000	11.012680000000000	7.428570000000000
O	10.975090000000000	11.063840000000001	9.325970000000000
O	9.496390000000000	16.310590000000001	6.503950000000000
O	7.590730000000000	14.315009999999999	6.420470000000000
O	12.479410000000000	5.697120000000000	6.482250000000000
O	14.418220000000000	7.681730000000000	6.551720000000000
O	9.504379999999999	5.648130000000000	7.079600000000000
O	12.492730000000000	16.365420000000000	7.073200000000000
O	7.635200000000000	7.577580000000000	7.687630000000000
O	16.284300000000002	12.504940000000000	7.580110000000000
O	16.346620000000001	9.563510000000001	7.006620000000000
O	14.344540000000000	14.440000000000000	7.717030000000000
O	5.649820000000000	12.431910000000000	6.810230000000000
O	5.700040000000000	9.505170000000000	7.458270000000000
N	11.015100000000000	13.034689999999999	7.089370000000000
N	10.980010000000000	8.979990000000001	7.117870000000000
N	12.990349999999999	11.029570000000000	7.110510000000000
N	9.004230000000000	10.982699999999999	7.078350000000000

Transition Metal: Fe; Functional Group: OH; Adsorbate: OOH

H	9.410670000000000	16.844500000000000	7.258210000000000
H	7.997890000000000	15.208240000000000	6.268240000000000
H	12.394959999999999	5.434350000000000	5.467860000000000
H	14.025740000000001	6.774280000000000	6.502170000000000
H	10.097130000000000	4.865890000000000	6.902070000000000
H	11.980700000000001	17.107710000000001	6.591980000000000
H	6.731930000000000	7.964150000000000	7.558620000000000
H	17.114200000000000	11.987990000000000	7.350890000000000
H	16.069620000000000	8.635999999999999	6.740530000000000
H	15.255179999999999	14.048920000000001	7.594650000000000
H	5.938400000000000	13.348699999999999	6.529470000000000
H	4.882140000000000	10.009720000000000	7.188790000000000
H	10.408030000000000	9.332060000000000	9.536210000000001
C	10.330840000000000	15.210870000000000	6.705430000000000
C	9.922680000000000	13.839219999999999	6.739860000000000
C	8.596970000000001	13.394909999999999	6.619320000000000
C	11.655090000000000	6.807720000000000	6.648900000000000
C	12.077199999999999	8.172010000000000	6.750910000000000
C	13.408950000000001	8.607170000000000	6.690910000000000
C	10.304330000000000	6.755940000000000	6.931360000000000
C	9.883200000000000	8.121490000000000	7.133110000000000
C	11.692110000000000	15.254460000000000	6.931210000000000
C	8.555410000000000	8.553020000000000	7.320790000000000
C	15.210270000000000	11.671400000000000	7.242410000000000
C	12.113470000000000	13.885120000000001	7.105810000000000
C	13.841519999999999	12.113340000000001	7.223680000000000
C	15.217320000000001	10.318059999999999	6.997390000000000
C	13.835310000000000	9.925829999999999	6.873610000000000
C	13.439230000000000	13.457400000000000	7.313110000000000
C	6.787090000000000	11.680870000000001	6.877840000000000
C	8.170280000000000	12.078010000000001	6.805300000000000
C	6.788190000000000	10.334740000000000	7.162540000000000
C	8.157170000000001	9.897560000000000	7.208840000000000
Fe	10.996499999999999	11.013320000000000	7.267850000000000
O	9.490740000000001	16.310659999999999	6.443500000000000
O	7.589710000000000	14.315580000000001	6.347650000000000
O	12.486599999999999	5.694870000000000	6.405480000000000
O	14.424720000000001	7.673990000000000	6.491520000000000
O	9.510350000000001	5.644270000000000	6.975710000000000
O	12.492160000000000	16.364529999999998	6.967440000000000
O	7.628270000000000	7.567390000000000	7.545130000000000
O	16.293849999999999	12.507840000000000	7.441160000000000
O	16.355290000000000	9.559150000000001	6.909560000000000
O	14.359280000000000	14.444550000000000	7.550920000000000
O	5.650880000000000	12.431350000000000	6.725200000000000
O	5.699620000000000	9.499840000000001	7.341040000000000
O	11.049880000000000	11.110670000000001	9.210270000000000
O	10.357740000000000	10.162300000000000	10.059939999999999
N	11.021409999999999	13.029830000000000	6.980720000000000
N	10.981660000000000	8.980169999999999	7.028860000000000
N	12.997840000000000	11.028720000000000	7.004030000000000
N	9.007000000000000	10.982139999999999	6.999910000000000

Transition Metal: Mn; Functional Group: BH2; Adsorbate: Clean

H	8.269670000000000	16.583310000000001	6.240410000000000
H	10.004830000000000	17.610830000000000	6.696650000000000
H	6.224690000000000	13.770880000000000	8.479279999999999
H	6.767210000000000	15.415740000000000	7.477710000000000
H	11.715840000000000	4.387480000000000	6.812130000000000
H	13.416550000000001	5.398190000000000	6.212710000000000
H	14.890390000000000	6.593460000000000	7.428720000000000
H	15.646269999999999	8.233180000000001	6.509570000000000
H	8.972590000000000	4.909660000000000	8.187070000000000
H	8.731949999999999	5.161020000000000	6.152490000000000
H	13.698850000000000	15.572880000000000	6.132660000000000
H	12.921120000000000	17.288580000000000	6.896260000000000
H	6.198470000000000	7.728660000000000	7.552830000000000
H	7.624100000000000	6.274730000000000	7.509030000000000
H	16.420310000000001	13.461570000000000	8.583090000000000
H	17.483360000000001	11.954650000000001	7.640500000000000
H	15.485870000000000	8.224259999999999	8.430280000000000
H	17.175329999999999	8.991370000000000	7.606050000000000
H	13.664859999999999	15.785539999999999	8.047129999999999
H	15.297890000000001	14.981100000000000	7.181140000000000
H	4.529380000000000	12.977240000000000	7.677250000000000
H	6.041260000000000	13.764490000000000	6.561000000000000
H	4.850420000000000	8.944310000000000	6.634630000000000
H	5.011220000000000	8.941350000000000	8.692620000000000
B	9.397190000000000	16.571069999999999	6.650970000000000
B	6.942570000000000	14.235870000000000	7.439570000000000
B	12.320390000000000	5.426710000000000	6.700470000000000
B	14.737240000000000	7.776070000000000	7.397110000000000
B	9.125980000000000	5.598530000000000	7.206960000000000
B	12.831320000000000	16.102550000000001	7.025170000000000
B	7.416800000000000	7.492850000000000	7.490240000000000
B	16.427000000000000	12.457910000000000	7.923640000000000
B	15.984310000000001	9.061520000000000	7.512140000000000
B	14.108990000000000	14.859090000000000	7.189550000000000
B	5.720370000000000	12.917249999999999	7.567590000000000
B	5.503610000000000	9.200070000000000	7.619180000000000
Mn	10.868470000000000	11.012050000000000	7.326900000000000
C	10.139960000000000	15.281820000000000	7.039250000000000
C	9.664440000000001	13.903729999999999	7.195370000000000
C	8.326070000000000	13.438070000000000	7.317560000000000
C	11.595120000000000	6.718050000000000	7.104860000000000
C	12.051069999999999	8.108430000000000	7.203470000000000
C	13.369930000000000	8.593109999999999	7.292780000000000
C	10.188350000000000	6.763220000000000	7.228810000000000
C	9.832630000000000	8.146660000000001	7.324030000000000
C	11.550079999999999	15.190270000000000	7.100730000000000
C	8.475310000000000	8.547319999999999	7.420730000000000
C	15.127359999999999	11.723860000000000	7.523890000000000
C	11.886139999999999	13.816750000000001	7.235350000000000
C	13.732440000000000	12.192420000000000	7.420120000000000
C	15.056229999999999	10.330840000000000	7.455340000000000
C	13.660190000000000	9.970330000000001	7.367060000000000
C	13.265150000000000	13.502440000000000	7.314840000000000
C	6.661730000000000	11.665020000000000	7.508300000000000
C	8.050200000000000	12.075460000000000	7.400320000000000
C	6.651680000000000	10.275340000000000	7.530260000000000
C	8.060390000000000	9.886939999999999	7.443620000000000
N	10.750410000000000	13.020099999999999	7.283690000000000
N	10.944459999999999	8.972680000000000	7.300520000000000
N	12.854780000000000	11.091740000000000	7.349190000000000
N	8.902740000000000	10.974320000000001	7.371820000000000

Transition Metal: Mn; Functional Group: BH2; Adsorbate: O

C	10.147340000000000	15.287330000000001	6.746390000000000
C	9.671889999999999	13.895250000000001	6.876110000000000
C	8.336110000000000	13.431749999999999	6.937100000000000
C	11.581080000000000	6.708160000000000	6.818230000000000
C	12.040960000000000	8.112620000000000	6.889220000000000
C	13.352029999999999	8.598800000000001	6.919570000000000
C	10.189650000000000	6.753510000000000	6.971810000000000
C	9.839079999999999	8.157719999999999	7.056110000000000
C	11.543270000000000	15.203989999999999	6.845310000000000
C	8.481460000000000	8.548299999999999	7.139320000000000
C	15.141890000000000	11.720549999999999	7.103480000000000
C	11.884499999999999	13.816260000000000	6.972200000000000
C	13.740240000000000	12.192170000000001	7.079900000000000
C	15.054620000000000	10.327780000000001	7.004150000000000
C	13.655920000000000	9.982370000000000	6.979010000000000
C	13.261030000000000	13.510619999999999	7.034810000000000
C	6.656270000000000	11.666720000000000	7.061090000000000
C	8.049770000000001	12.066950000000000	7.006650000000000
C	6.639630000000000	10.277469999999999	7.115610000000000
C	8.055840000000000	9.889310000000000	7.097720000000000
B	9.420389999999999	16.580549999999999	6.326440000000000
B	6.948070000000000	14.239039999999999	6.985220000000000
B	12.288140000000000	5.409540000000000	6.392010000000000
B	14.724050000000000	7.771870000000000	6.946480000000000
B	9.097080000000000	5.612500000000000	6.959050000000000
B	12.822780000000000	16.122660000000000	6.794170000000000
B	7.444780000000000	7.474000000000000	7.247120000000000
B	16.468029999999999	12.431660000000001	7.448430000000000
B	15.975120000000000	9.050110000000000	7.002880000000000
B	14.096579999999999	14.878349999999999	6.938630000000000
B	5.720500000000000	12.927759999999999	7.065810000000000
B	5.480220000000000	9.215920000000001	7.173070000000000
H	8.354570000000001	16.580269999999999	5.774850000000000
H	9.985569999999999	17.630450000000000	6.494850000000000
H	6.184160000000000	13.794400000000000	7.993730000000000
H	6.781950000000000	15.421239999999999	6.995280000000000
H	11.717779999999999	4.367320000000000	6.600990000000000
H	13.330600000000000	5.383520000000000	5.798100000000000
H	14.865930000000001	6.587480000000000	6.955190000000000
H	15.581730000000000	8.223290000000000	6.013810000000000
H	8.987890000000000	4.883950000000000	7.916780000000000
H	8.680479999999999	5.199330000000000	5.902410000000000
H	13.689090000000000	15.618220000000001	5.893970000000000
H	12.904360000000000	17.311630000000001	6.693800000000000
H	6.227530000000000	7.680810000000000	7.289910000000000
H	7.687360000000000	6.260860000000000	7.357890000000000
H	16.513710000000000	13.466740000000000	8.053280000000001
H	17.499810000000000	11.875810000000000	7.172290000000000
H	15.520880000000000	8.201150000000000	7.941150000000000
H	17.168119999999998	8.970990000000000	7.037040000000000
H	13.642659999999999	15.786630000000001	7.813650000000000
H	15.282530000000000	15.011350000000000	6.941720000000000
H	4.526310000000000	12.997150000000000	7.122380000000000
H	6.089960000000000	13.768470000000001	6.067920000000000
H	4.934360000000000	8.866250000000001	6.153730000000000
H	4.908750000000000	9.003330000000000	8.215630000000001
Mn	10.866199999999999	11.026050000000000	7.290800000000000
O	10.894959999999999	11.027990000000001	8.961349999999999
N	10.753780000000001	13.024419999999999	6.988200000000000
N	10.939489999999999	8.970670000000000	7.004480000000000
N	12.867699999999999	11.104229999999999	7.013870000000000
N	8.890620000000000	10.971030000000001	7.022380000000000

Transition Metal: Mn; Functional Group: BH2; Adsorbate: OH

C	10.147550000000001	15.299709999999999	6.646740000000000
C	9.671160000000000	13.909280000000001	6.768070000000000
C	8.333430000000000	13.438580000000000	6.817010000000000
C	11.582150000000000	6.705360000000000	6.707530000000000
C	12.045140000000000	8.108269999999999	6.776880000000000
C	13.353870000000001	8.599890000000000	6.801520000000000
C	10.190110000000001	6.754070000000000	6.870420000000000
C	9.843340000000000	8.159829999999999	6.961780000000000
C	11.546820000000000	15.216320000000000	6.731320000000000
C	8.483020000000000	8.549220000000000	7.050040000000000
C	15.147220000000001	11.727000000000000	6.995010000000000
C	11.888230000000000	13.829370000000001	6.847420000000000
C	13.747000000000000	12.200440000000000	6.958000000000000
C	15.056260000000000	10.332150000000000	6.901580000000000
C	13.658960000000000	9.986980000000001	6.868180000000000
C	13.265850000000000	13.518700000000001	6.901370000000000
C	6.657530000000000	11.670880000000000	6.937080000000000
C	8.048050000000000	12.074769999999999	6.888830000000000
C	6.646570000000000	10.279949999999999	7.009620000000000
C	8.064399999999999	9.896970000000000	7.004970000000000
B	9.420859999999999	16.600840000000002	6.247470000000000
B	6.940990000000000	14.242940000000001	6.846730000000000
B	12.288869999999999	5.402830000000000	6.290960000000000
B	14.727330000000000	7.775360000000000	6.823340000000000
B	9.085319999999999	5.622920000000000	6.864050000000000
B	12.826020000000000	16.132670000000001	6.667920000000000
B	7.446730000000000	7.483410000000000	7.149100000000000
B	16.470199999999998	12.438710000000000	7.345080000000000
B	15.977259999999999	9.053979999999999	6.895400000000000
B	14.101910000000000	14.886200000000001	6.793980000000000
B	5.717680000000000	12.927569999999999	6.923160000000000
B	5.499660000000000	9.202769999999999	7.077470000000000
H	10.750510000000000	11.766529999999999	9.610970000000000
H	8.358800000000000	16.610479999999999	5.689660000000000
H	9.984040000000000	17.647739999999999	6.440020000000000
H	6.167090000000000	13.806780000000000	7.849520000000000
H	6.772670000000000	15.424950000000001	6.845990000000000
H	11.709190000000000	4.364170000000000	6.490120000000000
H	13.340579999999999	5.369910000000000	5.714630000000000
H	14.872230000000000	6.591560000000000	6.818210000000000
H	15.586580000000000	8.238260000000000	5.897310000000000
H	8.977539999999999	4.899090000000000	7.825680000000000
H	8.683350000000001	5.197030000000000	5.807240000000000
H	13.680630000000001	15.625460000000000	5.755910000000000
H	12.909700000000001	17.321480000000001	6.565560000000000
H	6.225590000000000	7.696510000000000	7.187980000000000
H	7.680820000000000	6.265570000000000	7.249970000000000
H	16.513480000000001	13.494560000000000	7.913270000000000
H	17.502459999999999	11.865050000000000	7.109430000000000
H	15.520659999999999	8.197050000000001	7.824260000000000
H	17.170059999999999	8.974480000000000	6.932810000000000
H	13.660840000000000	15.794440000000000	7.675790000000000
H	15.287750000000001	15.018890000000001	6.779280000000000
H	4.523090000000000	12.993819999999999	6.963850000000000
H	6.096430000000000	13.766670000000000	5.923410000000000
H	4.934720000000000	8.865539999999999	6.063950000000000
H	4.931040000000000	9.003590000000001	8.125040000000000
Mn	10.875930000000000	11.032019999999999	7.217490000000000
O	10.894660000000000	10.935180000000001	9.122949999999999
N	10.753790000000000	13.039040000000000	6.875180000000000
N	10.941760000000000	8.965320000000000	6.906220000000000
N	12.873329999999999	11.110020000000000	6.894470000000000
N	8.891950000000000	10.974410000000001	6.925780000000000

Transition Metal: Mn; Functional Group: BH2; Adsorbate: OOH

Mn	10.866199999999999	11.026050000000000	7.290800000000000
C	10.147340000000000	15.287330000000001	6.746390000000000
C	9.671889999999999	13.895250000000001	6.876110000000000
C	8.336110000000000	13.431749999999999	6.937100000000000
C	11.581080000000000	6.708160000000000	6.818230000000000
C	12.040960000000000	8.112620000000000	6.889220000000000
C	13.352029999999999	8.598800000000001	6.919570000000000
C	10.189650000000000	6.753510000000000	6.971810000000000
C	9.839079999999999	8.157719999999999	7.056110000000000
C	11.543270000000000	15.203989999999999	6.845310000000000
C	8.481460000000000	8.548299999999999	7.139320000000000
C	15.141890000000000	11.720549999999999	7.103480000000000
C	11.884499999999999	13.816260000000000	6.972200000000000
C	13.740240000000000	12.192170000000001	7.079900000000000
C	15.054620000000000	10.327780000000001	7.004150000000000
C	13.655920000000000	9.982370000000000	6.979010000000000
C	13.261030000000000	13.510619999999999	7.034810000000000
C	6.656270000000000	11.666720000000000	7.061090000000000
C	8.049770000000001	12.066950000000000	7.006650000000000
C	6.639630000000000	10.277469999999999	7.115610000000000
C	8.055840000000000	9.889310000000000	7.097720000000000
B	9.420389999999999	16.580549999999999	6.326440000000000
B	6.948070000000000	14.239039999999999	6.985220000000000
B	12.288140000000000	5.409540000000000	6.392010000000000
B	14.724050000000000	7.771870000000000	6.946480000000000
B	9.097080000000000	5.612500000000000	6.959050000000000
B	12.822780000000000	16.122660000000000	6.794170000000000
B	7.444780000000000	7.474000000000000	7.247120000000000
B	16.468029999999999	12.431660000000001	7.448430000000000
B	15.975120000000000	9.050110000000000	7.002880000000000
B	14.096579999999999	14.878349999999999	6.938630000000000
B	5.720500000000000	12.927759999999999	7.065810000000000
B	5.480220000000000	9.215920000000001	7.173070000000000
H	8.354570000000001	16.580269999999999	5.774850000000000
H	9.985569999999999	17.630450000000000	6.494850000000000
H	6.184160000000000	13.794400000000000	7.993730000000000
H	6.781950000000000	15.421239999999999	6.995280000000000
H	11.717779999999999	4.367320000000000	6.600990000000000
H	13.330600000000000	5.383520000000000	5.798100000000000
H	14.865930000000001	6.587480000000000	6.955190000000000
H	15.581730000000000	8.223290000000000	6.013810000000000
H	8.987890000000000	4.883950000000000	7.916780000000000
H	8.680479999999999	5.199330000000000	5.902410000000000
H	13.689090000000000	15.618220000000001	5.893970000000000
H	12.904360000000000	17.311630000000001	6.693800000000000
H	6.227530000000000	7.680810000000000	7.289910000000000
H	7.687360000000000	6.260860000000000	7.357890000000000
H	16.513710000000000	13.466740000000000	8.053280000000001
H	17.499810000000000	11.875810000000000	7.172290000000000
H	15.520880000000000	8.201150000000000	7.941150000000000
H	17.168119999999998	8.970990000000000	7.037040000000000
H	13.642659999999999	15.786630000000001	7.813650000000000
H	15.282530000000000	15.011350000000000	6.941720000000000
H	4.526310000000000	12.997150000000000	7.122380000000000
H	6.089960000000000	13.768470000000001	6.067920000000000
H	4.934360000000000	8.866250000000001	6.153730000000000
H	4.908750000000000	9.003330000000000	8.215630000000001
N	10.753780000000001	13.024419999999999	6.988200000000000
N	10.939489999999999	8.970670000000000	7.004480000000000
N	12.867699999999999	11.104229999999999	7.013870000000000
N	8.890620000000000	10.971030000000001	7.022380000000000
O	10.900626649332507	11.028372242687938	9.290502331099464
H	10.079233067545946	10.871608475187058	10.987059327597715
O	9.683003769601120	10.796635707491451	10.099593253199657

Transition Metal: Mn; Functional Group: CH3; Adsorbate: Clean

H	9.151660000000000	16.223569999999999	9.058410000000000
H	10.619470000000000	17.113130000000002	8.646649999999999
H	9.270569999999999	17.077739999999999	7.506150000000000
H	6.598550000000000	14.224679999999999	7.290450000000000
H	7.232090000000000	14.857360000000000	8.819870000000000
H	7.854370000000000	15.440659999999999	7.266940000000000
H	12.464510000000001	5.643250000000000	9.697089999999999
H	11.946249999999999	4.789010000000000	8.236230000000001
H	13.432580000000000	5.736520000000000	8.216329999999999
H	14.818400000000000	8.742060000000000	10.021870000000000
H	13.538449999999999	7.547370000000000	10.204730000000000
H	14.810380000000000	7.293740000000000	9.000220000000001
H	9.476920000000000	5.296560000000000	6.246970000000000
H	10.012680000000000	4.749990000000000	7.842790000000000
H	8.534990000000001	5.699200000000000	7.692250000000000
H	12.265190000000000	17.236429999999999	7.492210000000000
H	13.666169999999999	16.166530000000002	7.324310000000000
H	12.766700000000000	16.693049999999999	5.890630000000000
H	8.477309999999999	7.096410000000000	5.283650000000000
H	7.194240000000000	7.027180000000000	6.501130000000000
H	7.179800000000000	8.288270000000001	5.255690000000000
H	16.404859999999999	13.363390000000001	6.862710000000000
H	17.307530000000000	11.848250000000000	6.908090000000000
H	16.493169999999999	12.345030000000000	5.416900000000000
H	16.630610000000001	9.672929999999999	9.158460000000000
H	16.279750000000000	8.556139999999999	7.829380000000000
H	17.272600000000001	9.986319999999999	7.539340000000000
H	14.892799999999999	14.774830000000000	5.976110000000000
H	14.702760000000000	13.485010000000001	4.776160000000000
H	13.503150000000000	14.771080000000000	4.878560000000000
H	4.852020000000000	11.534030000000000	8.672090000000001
H	5.802280000000000	12.958500000000001	9.102950000000000
H	4.980450000000000	12.878050000000000	7.532320000000000
H	5.771990000000000	8.431850000000001	7.633020000000000
H	4.720820000000000	9.858660000000000	7.613600000000000
H	5.319240000000000	9.188490000000000	6.096290000000000
C	10.448740000000001	15.226400000000000	7.623400000000000
C	9.933550000000000	13.873070000000000	7.612900000000000
C	8.574220000000000	13.456289999999999	7.763700000000000
C	11.610090000000000	6.919470000000000	8.138120000000001
C	12.006959999999999	8.312030000000000	8.154030000000001
C	13.291550000000001	8.836840000000000	8.493040000000001
C	10.365360000000001	6.853790000000000	7.501910000000000
C	9.973129999999999	8.213020000000000	7.199640000000000
C	11.738500000000000	15.183059999999999	7.084140000000000
C	8.690659999999999	8.656660000000000	6.757130000000000
C	15.165210000000000	11.583990000000000	6.976530000000000
C	12.049510000000000	13.794210000000000	6.848380000000000
C	13.769740000000001	12.012940000000000	6.845110000000000
C	15.163660000000000	10.416090000000001	7.717350000000000
C	13.764150000000001	10.052390000000001	7.955690000000000
C	13.311780000000001	13.272330000000000	6.418330000000000
C	6.771350000000000	11.613630000000001	7.697200000000000
C	8.152390000000000	12.113759999999999	7.677470000000000
C	6.797820000000000	10.310510000000001	7.240380000000000
C	8.203220000000000	9.944010000000000	7.065120000000000
C	9.832770000000000	16.464169999999999	8.232630000000000
C	7.511290000000000	14.548060000000000	7.797960000000000
C	12.401360000000000	5.720300000000000	8.598680000000000
C	14.167080000000000	8.058700000000000	9.464530000000000
C	9.559659999999999	5.593690000000000	7.305600000000000
C	12.655799999999999	16.370509999999999	6.939720000000000
C	7.833410000000000	7.714120000000000	5.923770000000000
C	16.397349999999999	12.319480000000000	6.514690000000000
C	16.391510000000000	9.620410000000000	8.083110000000000
C	14.154790000000000	14.124100000000000	5.479880000000000

C	5.547530000000000	12.287080000000000	8.272779999999999
C	5.600540000000000	9.401090000000000	7.140910000000000
Mn	10.970610000000001	11.046010000000001	7.382650000000000
N	10.966450000000000	13.013109999999999	7.224890000000000
N	10.990159999999999	9.074140000000000	7.590050000000000
N	12.942629999999999	11.041350000000000	7.413660000000000
N	9.005720000000000	11.037850000000001	7.392100000000000

Transition Metal: Mn; Functional Group: CH3; Adsorbate: O

H	9.256800000000000	16.170470000000002	9.143720000000000
H	10.684010000000001	17.090109999999999	8.657730000000001
H	9.268070000000000	17.048810000000000	7.600670000000000
H	6.622530000000000	14.212859999999999	7.390890000000000
H	7.295260000000000	14.785940000000000	8.927149999999999
H	7.871050000000000	15.437260000000000	7.382210000000000
H	12.362679999999999	5.732090000000000	9.784210000000000
H	11.881330000000000	4.811440000000000	8.351050000000001
H	13.378100000000000	5.745270000000000	8.331780000000000
H	14.734710000000000	8.803970000000000	10.045360000000001
H	13.468420000000000	7.592450000000000	10.212759999999999
H	14.770680000000000	7.347470000000000	9.037080000000000
H	9.490629999999999	5.316210000000000	6.187020000000000
H	9.999720000000000	4.749680000000000	7.785850000000000
H	8.524770000000000	5.704610000000000	7.620340000000000
H	12.278740000000001	17.232749999999999	7.430830000000000
H	13.673710000000000	16.154499999999999	7.251110000000000
H	12.756840000000000	16.673559999999998	5.826530000000000
H	8.477420000000000	7.091910000000000	5.204980000000000
H	7.181400000000000	7.060720000000000	6.415020000000000
H	7.205800000000000	8.312020000000000	5.158450000000000
H	16.392360000000000	13.394890000000000	6.908090000000000
H	17.302510000000002	11.883960000000000	6.958000000000000
H	16.507169999999999	12.385479999999999	5.456990000000000
H	16.572479999999999	9.754250000000001	9.250400000000001
H	16.282319999999999	8.602700000000000	7.934500000000000
H	17.261920000000000	10.041430000000000	7.645950000000000
H	14.902590000000000	14.732279999999999	5.902870000000000
H	14.671350000000000	13.454129999999999	4.696820000000000
H	13.503240000000000	14.769140000000000	4.813770000000000
H	4.911940000000000	11.481550000000000	8.768560000000001
H	5.867740000000000	12.901070000000001	9.202859999999999
H	5.004400000000000	12.849069999999999	7.652410000000000
H	5.787830000000000	8.412100000000001	7.640970000000000
H	4.738220000000000	9.840040000000000	7.631640000000000
H	5.333440000000000	9.176690000000001	6.108620000000000
C	10.478030000000000	15.215590000000001	7.618340000000000
C	9.957739999999999	13.847700000000000	7.601260000000000
C	8.610080000000000	13.436500000000001	7.780600000000000
C	11.569150000000000	6.935950000000000	8.141790000000000
C	11.976889999999999	8.341320000000000	8.122370000000000
C	13.247070000000001	8.863060000000001	8.480499999999999
C	10.359000000000000	6.855890000000000	7.464860000000000
C	9.974380000000000	8.221750000000000	7.123300000000000
C	11.739000000000001	15.179950000000000	7.039680000000000
C	8.704650000000001	8.658210000000000	6.667320000000000
C	15.160500000000001	11.607590000000000	6.985460000000000
C	12.047169999999999	13.779620000000000	6.786340000000000
C	13.769370000000000	12.007360000000000	6.796910000000000
C	15.144819999999999	10.444940000000001	7.745230000000000
C	13.741569999999999	10.078329999999999	7.935750000000000
C	13.297090000000001	13.263990000000000	6.344630000000000
C	6.801250000000000	11.589420000000000	7.740140000000000
C	8.176180000000000	12.088500000000000	7.674100000000000
C	6.813920000000000	10.291940000000000	7.248420000000000
C	8.207850000000001	9.946479999999999	7.005280000000000
C	9.883250000000000	16.435440000000000	8.282209999999999
C	7.547200000000000	14.522530000000000	7.885680000000000
C	12.335319999999999	5.754870000000000	8.681940000000001
C	14.105230000000001	8.105210000000000	9.481850000000000
C	9.555899999999999	5.598990000000000	7.250290000000000
C	12.659000000000001	16.362010000000001	6.879610000000000
C	7.840700000000000	7.725990000000000	5.834710000000000
C	16.396500000000000	12.352850000000000	6.552740000000000
C	16.369360000000000	9.673500000000001	8.169219999999999
C	14.144840000000000	14.105530000000000	5.406000000000000

C	5.592870000000000	12.245970000000000	8.365980000000000
C	5.615640000000000	9.384060000000000	7.153690000000000
Mn	10.972630000000001	11.021340000000000	7.024560000000000
O	10.997859999999999	10.867889999999999	5.356560000000000
N	10.982510000000000	12.999210000000000	7.192120000000000
N	10.976940000000001	9.084920000000000	7.517640000000000
N	12.945090000000000	11.048180000000000	7.354340000000000
N	9.006130000000001	11.029299999999999	7.320270000000000

Transition Metal: Mn; Functional Group: CH3; Adsorbate: OH

H	10.437490000000000	11.361610000000001	4.509080000000000
H	9.250529999999999	16.175460000000001	9.150280000000000
H	10.675850000000001	17.103909999999999	8.675890000000001
H	9.265850000000000	17.060730000000000	7.611760000000000
H	6.621100000000000	14.230240000000000	7.383060000000000
H	7.298520000000000	14.796960000000000	8.918900000000001
H	7.869780000000000	15.454150000000000	7.375600000000000
H	12.373490000000000	5.730670000000000	9.776270000000000
H	11.897290000000000	4.811510000000000	8.340710000000000
H	13.388620000000000	5.753600000000000	8.324750000000000
H	14.729419999999999	8.813040000000001	10.048069999999999
H	13.461770000000000	7.603520000000000	10.212100000000000
H	14.772130000000001	7.351840000000000	9.047359999999999
H	9.475330000000000	5.313320000000000	6.207520000000000
H	10.005870000000000	4.748380000000000	7.799980000000000
H	8.528029999999999	5.701500000000000	7.652900000000000
H	12.302920000000000	17.243770000000001	7.506990000000000
H	13.692710000000000	16.161290000000001	7.315080000000000
H	12.789289999999999	16.714469999999999	5.895110000000000
H	8.452819999999999	7.084030000000000	5.229710000000000
H	7.180100000000000	7.046870000000000	6.464070000000000
H	7.171400000000000	8.293830000000000	5.203940000000000
H	16.416519999999998	13.408030000000000	6.970330000000000
H	17.321719999999999	11.893549999999999	7.000380000000000
H	16.535080000000001	12.422140000000001	5.503790000000000
H	16.582239999999999	9.748710000000001	9.258520000000001
H	16.281800000000000	8.602259999999999	7.941140000000000
H	17.271740000000001	10.034000000000001	7.653580000000000
H	14.941670000000000	14.752370000000001	5.971400000000000
H	14.707970000000000	13.497650000000000	4.740820000000000
H	13.550730000000000	14.820480000000000	4.873520000000000
H	4.915570000000000	11.502780000000000	8.776890000000000
H	5.879110000000000	12.918910000000000	9.203139999999999
H	5.008620000000000	12.866930000000000	7.657650000000000
H	5.800160000000000	8.413550000000001	7.682440000000000
H	4.743760000000000	9.836000000000000	7.692970000000000
H	5.310070000000000	9.172810000000000	6.158960000000000
C	10.484010000000000	15.232120000000000	7.627790000000000
C	9.960160000000000	13.865420000000000	7.583270000000000
C	8.610830000000000	13.451499999999999	7.761220000000000
C	11.574769999999999	6.935920000000000	8.138249999999999
C	11.983079999999999	8.341609999999999	8.109680000000001
C	13.252760000000000	8.865869999999999	8.472200000000001
C	10.358180000000001	6.855060000000000	7.473140000000000
C	9.974110000000000	8.221480000000000	7.127150000000000
C	11.755660000000001	15.199940000000000	7.070570000000000
C	8.697609999999999	8.655960000000000	6.683500000000000
C	15.178360000000000	11.623849999999999	7.012110000000000
C	12.061150000000000	13.801740000000001	6.799380000000000
C	13.787110000000000	12.023370000000000	6.813450000000000
C	15.156560000000001	10.451140000000001	7.756330000000000
C	13.751180000000000	10.082269999999999	7.929660000000000
C	13.320440000000000	13.288760000000000	6.374930000000000
C	6.801540000000000	11.600490000000001	7.740490000000000
C	8.174960000000000	12.102029999999999	7.650980000000000
C	6.811200000000000	10.295650000000000	7.265730000000000
C	8.203080000000000	9.951960000000000	7.005140000000000
C	9.880620000000000	16.446950000000001	8.293410000000000
C	7.548080000000000	14.536720000000001	7.875910000000000
C	12.345920000000000	5.756470000000000	8.674250000000001
C	14.103640000000000	8.112349999999999	9.482950000000001
C	9.554280000000000	5.596890000000000	7.269610000000000
C	12.681880000000000	16.381699999999999	6.941010000000000
C	7.823880000000000	7.715590000000000	5.870200000000000
C	16.419129999999999	12.371880000000001	6.598280000000000
C	16.377120000000001	9.671760000000001	8.177420000000000

C	14.181990000000001	14.140660000000000	5.458630000000000
C	5.598090000000000	12.262790000000001	8.369410000000000
C	5.613570000000000	9.383710000000001	7.197620000000000
Mn	10.983470000000001	11.023990000000000	6.975170000000000
O	11.050200000000000	10.813200000000000	5.030100000000000
N	10.982550000000000	13.023660000000000	7.164260000000000
N	10.985390000000001	9.079800000000001	7.502880000000000
N	12.962550000000000	11.052490000000001	7.345220000000000
N	8.998060000000001	11.044910000000000	7.284050000000000

Transition Metal: Mn; Functional Group: CH3; Adsorbate: OOH

Mn	10.9726300000000001	11.0213400000000000	7.0245600000000000
H	9.2568000000000000	16.1704700000000002	9.1437200000000000
H	10.6840100000000001	17.0901099999999999	8.6577300000000001
H	9.2680700000000000	17.0488100000000000	7.6006700000000000
H	6.6225300000000000	14.2128599999999999	7.3908900000000000
H	7.2952600000000000	14.7859400000000000	8.9271499999999999
H	7.8710500000000000	15.4372600000000000	7.3822100000000000
H	12.3626799999999999	5.7320900000000000	9.7842100000000000
H	11.8813300000000000	4.8114400000000000	8.3510500000000001
H	13.3781000000000000	5.7452700000000000	8.3317800000000000
H	14.7347100000000000	8.8039700000000000	10.0453600000000001
H	13.4684200000000000	7.5924500000000000	10.2127599999999999
H	14.7706800000000000	7.3474700000000000	9.0370800000000000
H	9.4906299999999999	5.3162100000000000	6.1870200000000000
H	9.9997200000000000	4.7496800000000000	7.7858500000000000
H	8.5247700000000000	5.7046100000000000	7.6203400000000000
H	12.2787400000000001	17.2327499999999999	7.4308300000000000
H	13.6737100000000000	16.1544999999999999	7.2511100000000000
H	12.7568400000000000	16.6735599999999998	5.8265300000000000
H	8.4774200000000000	7.0919100000000000	5.2049800000000000
H	7.1814000000000000	7.0607200000000000	6.4150200000000000
H	7.2058000000000000	8.3120200000000000	5.1584500000000000
H	16.3923600000000000	13.3948900000000000	6.9080900000000000
H	17.3025100000000002	11.8839600000000000	6.9580000000000000
H	16.5071699999999999	12.3854799999999999	5.4569900000000000
H	16.5724799999999999	9.7542500000000001	9.2504000000000001
H	16.2823199999999999	8.6027000000000000	7.9345000000000000
H	17.2619200000000000	10.0414300000000000	7.6459500000000000
H	14.9025900000000000	14.7322799999999999	5.9028700000000000
H	14.6713500000000000	13.4541299999999999	4.6968200000000000
H	13.5032400000000000	14.7691400000000000	4.8137700000000000
H	4.9119400000000000	11.4815500000000000	8.7685600000000001
H	5.8677400000000000	12.9010700000000001	9.2028599999999999
H	5.0044000000000000	12.8490699999999999	7.6524100000000000
H	5.7878300000000000	8.4121000000000001	7.6409700000000000
H	4.7382200000000000	9.8400400000000000	7.6316400000000000
H	5.3334400000000000	9.1766900000000001	6.1086200000000000
C	10.4780300000000000	15.2155900000000001	7.6183400000000000
C	9.9577399999999999	13.8477000000000000	7.6012600000000000
C	8.6100800000000000	13.4365000000000001	7.7806000000000000
C	11.5691500000000000	6.9359500000000000	8.1417900000000000
C	11.9768899999999999	8.3413200000000000	8.1223700000000000
C	13.2470700000000001	8.8630600000000001	8.4804999999999999
C	10.3590000000000000	6.8558900000000000	7.4648600000000000
C	9.9743800000000000	8.2217500000000000	7.1233000000000000
C	11.7390000000000001	15.1799500000000000	7.0396800000000000
C	8.7046500000000001	8.6582100000000000	6.6673200000000000
C	15.1605000000000001	11.6075900000000000	6.9854600000000000
C	12.0471699999999999	13.7796200000000000	6.7863400000000000
C	13.7693700000000000	12.0073600000000000	6.7969100000000000
C	15.1448199999999999	10.4449400000000001	7.7452300000000000
C	13.7415699999999999	10.0783299999999999	7.9357500000000000
C	13.2970900000000001	13.2639900000000000	6.3446300000000000
C	6.8012500000000000	11.5894200000000000	7.7401400000000000
C	8.1761800000000000	12.0885000000000000	7.6741000000000000
C	6.8139200000000000	10.2919400000000000	7.2484200000000000
C	8.2078500000000001	9.9464799999999999	7.0052800000000000
C	9.8832500000000000	16.4354400000000000	8.2822099999999999
C	7.5472000000000000	14.5225300000000000	7.8856800000000000
C	12.3353199999999999	5.7548700000000000	8.6819400000000001
C	14.1052300000000001	8.1052100000000000	9.4818500000000000
C	9.5558999999999999	5.5989900000000000	7.2502900000000000
C	12.6590000000000001	16.3620100000000001	6.8796100000000000
C	7.8407000000000000	7.7259900000000000	5.8347100000000000
C	16.3965000000000000	12.3528500000000000	6.5527400000000000
C	16.3693600000000000	9.6735000000000001	8.1692199999999999

C	14.144840000000000	14.105530000000000	5.406000000000000
C	5.592870000000000	12.245970000000000	8.365980000000000
C	5.615640000000000	9.384060000000000	7.153690000000000
N	10.982510000000000	12.999210000000000	7.192120000000000
N	10.976940000000001	9.084920000000000	7.517640000000000
N	12.945090000000000	11.048180000000000	7.354340000000000
N	9.006130000000001	11.029299999999999	7.320270000000000
O	11.002751173208889	10.838141663539274	5.033195873466999
H	10.171573371660894	10.562057754458092	3.356744539628560
O	9.773597773550016	10.592012928066991	4.246088520625584

Transition Metal: Mn; Functional Group: F; Adsorbate: Clean

Mn	0.000000000000000	-0.000251796888862	0.002707265659100
C	0.688224806937092	4.249569256518612	-0.013277520353036
C	1.112791825817610	2.880438176170226	-0.001783429037472
C	2.438817356344596	2.431680916899768	0.005214186513566
C	-0.688229181525621	-4.249626561338014	0.003057951942570
C	-1.112809767930781	-2.880452343758144	-0.003466962191926
C	-2.438876303182951	-2.431563462201243	-0.005339698121082
C	0.688229181525622	-4.249626561338014	0.003057951942570
C	1.112809767930788	-2.880452343758144	-0.003466962191926
C	-0.688224806937093	4.249569256518612	-0.013277520353036
C	2.438876303182954	-2.431563462201243	-0.005339698121082
C	-4.255182387904519	0.683253003751122	0.011989604048168
C	-1.112791825817606	2.880438176170226	-0.001783429037472
C	-2.876088852521246	1.112730020485004	0.013389042103650
C	-4.255185760708748	-0.683254792954965	-0.006209415868064
C	-2.876062244025931	-1.112535106866719	-0.007422862793292
C	-2.438817356344586	2.431680916899768	0.005214186513566
C	4.255182387904522	0.683253003751122	0.011989604048168
C	2.876088852521254	1.112730020485004	0.013389042103650
C	4.255185760708752	-0.683254792954965	-0.006209415868064
C	2.876062244025934	-1.112535106866719	-0.007422862793292
N	0.000000000000000	2.038518720267614	0.005254047158214
N	0.000000000000000	-2.038581071865035	-0.007546750362456
N	-2.028137715606256	0.000098158343610	0.003815092223122
N	2.028137715606254	0.000098158343610	0.003815092223122
F	5.340690413110972	-1.477223075173693	-0.019572939334296
F	-5.340592438811822	1.477384252780666	0.019629209647448
F	-5.340690413110964	-1.477223075173693	-0.019572939334296
F	-1.474023331735900	5.341037560074872	-0.007286894138868
F	1.474023331735904	5.341037560074872	-0.007286894138868
F	5.340592438811834	1.477384252780666	0.019629209647448
F	-1.474290447352129	-5.341061454097527	-0.003548376874953
F	1.474290447352128	-5.341061454097527	-0.003548376874953
F	-3.401515247807666	3.398285030314272	-0.003487779075304
F	3.401515247807668	3.398285030314272	-0.003487779075304
F	-3.401341109870827	-3.398392504704610	0.000938510082096
F	3.401341109870830	-3.398392504704610	0.000938510082096

Transition Metal: Mn; Functional Group: F; Adsorbate: O

Mn	0.000000000000000	-0.000643290750705	0.266228261181810
C	0.684988457622258	4.253290457843004	-0.003537817130560
C	1.109687397490298	2.874974619622840	-0.007194537532018
C	2.432534075461420	2.431028423789796	0.007289977542758
C	-0.684981925245463	-4.255246585004270	-0.005183575930658
C	-1.109723162829237	-2.876977372376377	-0.005960734721232
C	-2.432679983854499	-2.433345469734910	0.005571066950478
C	0.684981925245468	-4.255246585004270	-0.005183575930658
C	1.109723162829230	-2.876977372376377	-0.005960734721232
C	-0.684988457622261	4.253290457843004	-0.003537817130560
C	2.432679983854506	-2.433345469734910	0.005571066950478
C	-4.255651938781636	0.683930843659418	0.007169518810732
C	-1.109687397490291	2.874974619622840	-0.007194537532018
C	-2.877201481744727	1.108453577572882	0.001097703496414
C	-4.255738735504037	-0.686040814878414	0.006263477694762
C	-2.877361025817994	-1.110768730498339	-0.000152622900484
C	-2.432534075461422	2.431028423789796	0.007289977542758
C	4.255651938781630	0.683930843659418	0.007169518810732
C	2.877201481744726	1.108453577572882	0.001097703496414
C	4.255738735504030	-0.686040814878414	0.006263477694762
C	2.877361025817990	-1.110768730498339	-0.000152622900484
N	0.000000000000000	2.039002013297378	-0.025948081935804
N	0.000000000000000	-2.040801684299641	-0.021751625697419
N	-2.041339490181432	-0.001201777684370	-0.018306386576420
N	2.041339490181430	-0.001201777684370	-0.018306386576420
F	5.340541477415046	-1.478687870507308	-0.001390355161913
F	-5.340311809194386	1.476732405590350	-0.000204191881231
F	-5.340541477415044	-1.478687870507308	-0.001390355161913
F	-1.477676822145352	5.338034503272442	-0.007842316537616
F	1.477676822145354	5.338034503272442	-0.007842316537616
F	5.340311809194383	1.476732405590350	-0.000204191881231
F	-1.477652569811461	-5.339962479571964	-0.012335585561033
F	1.477652569811464	-5.339962479571964	-0.012335585561033
F	-3.394574636829773	3.393677537250164	0.023534549236712
F	3.394574636829776	3.393677537250164	0.023534549236712
F	-3.394663044531246	-3.396193828256333	0.017156365378620
F	3.394663044531242	-3.396193828256333	0.017156365378620
O	0.000000000000000	0.005428081575976	1.938392376096228

Transition Metal: Mn; Functional Group: F; Adsorbate: OH

Mn	0.000000000000000	-0.025401491664304	0.348277197344202
C	0.686848060080948	4.310044786053208	-0.058084626464172
C	1.108044602433900	2.928297565246696	-0.038622678393556
C	2.423983079059576	2.449345367301642	-0.007400651801596
C	-0.686534151482736	-4.302873675933434	-0.057257617082115
C	-1.108933055984579	-2.922124708727313	-0.051667466907926
C	-2.425758385807406	-2.448100977992983	-0.012522749977640
C	0.686534151482728	-4.302873675933434	-0.057257617082115
C	1.108933055984572	-2.922124708727313	-0.051667466907926
C	-0.686848060080955	4.310044786053208	-0.058084626464172
C	2.425758385807400	-2.448100977992983	-0.012522749977640
C	-4.233274315755533	0.687119021481676	0.014242656022204
C	-1.108044602433903	2.928297565246696	-0.038622678393556
C	-2.856542420760295	1.116743113065732	0.013553470270282
C	-4.235507122887388	-0.684998055917337	0.015056676207312
C	-2.860224081500142	-1.116757559193374	0.012344889723650
C	-2.423983079059589	2.449345367301642	-0.007400651801596
C	4.233274315755534	0.687119021481676	0.014242656022204
C	2.856542420760304	1.116743113065732	0.013553470270282
C	4.235507122887392	-0.684998055917337	0.015056676207312
C	2.860224081500144	-1.116757559193374	0.012344889723650
N	0.000000000000000	2.104125374642556	-0.029141285676706
N	0.000000000000000	-2.098096737725584	-0.056686186580510
N	-2.026142812792997	-0.001750113281666	0.004312072037640
N	2.026142812793008	-0.001750113281666	0.004312072037640
F	5.326799153803377	-1.468900441817002	-0.004474889054634
F	-5.322885714207517	1.473455616038426	-0.005751724106425
F	-5.326799153803385	-1.468900441817002	-0.004474889054634
F	-1.479496788635068	5.396869058122245	-0.061626609801429
F	1.479496788635070	5.396869058122245	-0.061626609801429
F	5.322885714207514	1.473455616038426	-0.005751724106425
F	-1.479510009296682	-5.388221804434178	-0.048892100984588
F	1.479510009296684	-5.388221804434178	-0.048892100984588
F	-3.404097444374695	3.396397664454212	-0.002328235837778
F	3.404097444374704	3.396397664454212	-0.002328235837778
F	-3.403185603983879	-3.396962084284006	-0.000710499290818
F	3.403185603983886	-3.396962084284006	-0.000710499290818
H	0.000000000000000	0.851414059299742	2.695795343334340
O	0.000000000000000	-0.010086744917250	2.241045102461210

Transition Metal: Mn; Functional Group: F; Adsorbate: OOH

Mn	-0.004219738249578	0.001520848006840	0.239557039510254
C	0.681853006873988	4.260788754609398	-0.018122899515443
C	1.108299980102416	2.881787857127482	-0.009521732093837
C	2.432105968904344	2.437346749454268	-0.002630720239678
C	-0.688352296104199	-4.258567291194552	-0.018066627431786
C	-1.114303093317435	-2.879324232961341	-0.011359141897799
C	-2.437882635681547	-2.433896888038596	-0.007015066564470
C	0.681863196847046	-4.258455041797246	-0.018386866208211
C	1.107961661970580	-2.879302049105551	-0.010325690885619
C	-0.688295805110172	4.260887125172528	-0.017743694688868
C	2.431563051698980	-2.434535070461177	-0.002888958717944
C	-4.262266893029610	0.687659286817590	-0.015275602741602
C	-1.114585053399967	2.881820655734224	-0.010440187607937
C	-2.886397456531803	1.112692822068372	-0.015214157545544
C	-4.262199340025063	-0.685084125318287	-0.015052470722028
C	-2.886195336776968	-1.110019253526442	-0.015477021785950
C	-2.438338246406122	2.436720483109896	-0.006593308802572
C	4.257768861588239	0.687735507154096	-0.005308972024320
C	2.881510917797730	1.113236510379982	-0.005180557309224
C	4.257651611486546	-0.685211588083991	-0.005033955047926
C	2.881248264022392	-1.110567952456563	-0.005336277817270
N	-0.003359159082994	2.049279776516104	-0.010034455446586
N	-0.003385791602666	-2.046640699669744	-0.011217792271129
N	-2.054191062494841	0.001453332320594	-0.020471619084124
N	2.050316105031164	0.001477955438868	-0.010209950051574
F	5.345478045987680	-1.474472549426359	-0.006895574552324
F	-5.349440228148666	1.477368803644698	-0.014836544759952
F	-5.349698380953033	-1.474545282637088	-0.013282533493228
F	-1.480764976257753	5.346461355252709	-0.028802224771386
F	1.474619091235896	5.346254147974604	-0.030567782128866
F	5.345292753061436	1.477163616545218	-0.008396650828995
F	-1.481433512367953	-5.343770918303134	-0.028344164655028
F	1.475249568379532	-5.343540589791239	-0.030242917783113
F	-3.401716442710118	3.399988011260026	-0.001476028098964
F	3.395758703446398	3.400870142791942	0.001384691278368
F	-3.400840489727553	-3.397538260515994	-0.000821520360918
F	3.394825904199940	-3.398401884019780	0.002326786541626
H	-0.675539155461337	-0.000988282929278	3.891229209269588
O	0.188711940789558	0.002407552114468	2.208012672119198
O	-1.047523610757491	-0.000038313148922	2.984782324298110

Transition Metal: Mn; Functional Group: H; Adsorbate: Clean

Mn	0.000000000000000	-0.000256665832882	0.001559194741198
C	0.690074908262702	4.238885217791569	-0.008235771297656
C	1.110692471169452	2.868077021011474	-0.005237122625186
C	2.444278194847208	2.434757746944662	-0.001276850102578
C	-0.690128352715639	-4.238653166911558	-0.005557387694893
C	-1.110803192518055	-2.867916866972095	-0.000917354124548
C	-2.444443097715105	-2.434653318883242	0.000163553252658
C	0.690128352715634	-4.238653166911558	-0.005557387694893
C	1.110803192518060	-2.867916866972095	-0.000917354124548
C	-0.690074908262702	4.238885217791569	-0.008235771297656
C	2.444443097715112	-2.434653318883242	0.000163553252658
C	-4.244063216145095	0.682345530422344	0.005470835713402
C	-1.110692471169443	2.868077021011474	-0.005237122625186
C	-2.857863458390472	1.111506065449546	0.003023743876926
C	-4.244272175490721	-0.682283959542669	0.005635280853796
C	-2.858181585841010	-1.111625285504164	0.003576251880926
C	-2.444278194847215	2.434757746944662	-0.001276850102578
C	4.244063216145094	0.682345530422344	0.005470835713402
C	2.857863458390470	1.111506065449546	0.003023743876926
C	4.244272175490726	-0.682283959542669	0.005635280853796
C	2.858181585841016	-1.111625285504164	0.003576251880926
N	0.000000000000000	2.027079971942764	-0.004506951822718
N	0.000000000000000	-2.027157391576701	0.001664454892760
N	-2.010208564864246	-0.000150006050926	0.002886001892466
N	2.010208564864248	-0.000150006050926	0.002886001892466
H	5.095528945789288	-1.360541698313561	0.005299113585172
H	-5.095089259581371	1.360802114062332	0.005101559041898
H	-5.095528945789283	-1.360541698313561	0.005299113585172
H	-1.364544634040730	5.093011396101535	-0.009175051261934
H	1.364544634040724	5.093011396101535	-0.009175051261934
H	5.095089259581370	1.360802114062332	0.005101559041898
H	-1.364716653562581	-5.092693341605582	-0.008887053278336
H	1.364716653562588	-5.092693341605582	-0.008887053278336
H	-3.218879116131799	3.204257403970874	-0.001504410931454
H	3.218879116131798	3.204257403970874	-0.001504410931454
H	-3.218377790079813	-3.204747809237023	-0.002878687686520
H	3.218377790079824	-3.204747809237023	-0.002878687686520

Transition Metal: Mn; Functional Group: H; Adsorbate: O

Mn	0.000000000000000	-0.001345529363192	0.293607129507628
C	0.684876897117038	4.243708702255150	-0.017832371221374
C	1.106681126442014	2.859700872798342	0.007887702542522
C	2.435316114545620	2.434592019891694	0.014906647931428
C	-0.684846373348513	-4.245386366307592	-0.018311440178966
C	-1.106737922225381	-2.861280223325821	0.004821517141104
C	-2.435365118201616	-2.436061103026866	0.014517584553882
C	0.684846373348514	-4.245386366307592	-0.018311440178966
C	1.106737922225378	-2.861280223325821	0.004821517141104
C	-0.684876897117039	4.243708702255150	-0.017832371221374
C	2.435365118201622	-2.436061103026866	0.014517584553882
C	-4.244811208073296	0.684173434664608	-0.005554719800390
C	-1.106681126442012	2.859700872798342	0.007887702542522
C	-2.860518076607477	1.105930490693288	0.012252645755958
C	-4.244803956877991	-0.685475742741922	-0.004863762837402
C	-2.860546389878355	-1.107379827824985	0.012631388695336
C	-2.435316114545614	2.434592019891694	0.014906647931428
C	4.244811208073304	0.684173434664608	-0.005554719800390
C	2.860518076607478	1.105930490693288	0.012252645755958
C	4.244803956877988	-0.685475742741922	-0.004863762837402
C	2.860546389878358	-1.107379827824985	0.012631388695336
N	0.000000000000000	2.024675221396462	0.012759360728584
N	0.000000000000000	-2.026537629759822	0.007400786430714
N	-2.025904922693794	-0.000717550384230	0.013084103731600
N	2.025904922693800	-0.000717550384230	0.013084103731600
H	5.097246563980428	-1.361927255785044	-0.019613149520477
H	-5.096992108342064	1.360973610449320	-0.021408263492123
H	-5.097246563980427	-1.361927255785044	-0.019613149520477
H	-1.361496087289371	5.095992134592646	-0.038345155292891
H	1.361496087289366	5.095992134592646	-0.038345155292891
H	5.096992108342063	1.360973610449320	-0.021408263492123
H	-1.361324384594102	-5.097781167612091	-0.035414722344957
H	1.361324384594100	-5.097781167612091	-0.035414722344957
H	-3.207151628233312	3.206536308283014	0.011097216615950
H	3.207151628233306	3.206536308283014	0.011097216615950
H	-3.207240591365849	-3.207870298115264	0.013292816580318
H	3.207240591365844	-3.207870298115264	0.013292816580318
O	0.000000000000000	-0.005868139281763	1.968806645613480

Transition Metal: Mn; Functional Group: H; Adsorbate: OH

Mn	0.000000000000000	0.001248816638884	0.323438239428694
C	0.685835156041520	4.254407395748069	-0.047999479150224
C	1.108487082213002	2.871591734365544	-0.001470075830382
C	2.438920371277262	2.441891644012002	-0.005277559529072
C	-0.685428350521281	-4.245812214192973	-0.027774546623036
C	-1.107397291389155	-2.861736931836067	0.007486353024570
C	-2.437795505716277	-2.433008376793065	0.007553225678890
C	0.685428350521278	-4.245812214192973	-0.027774546623036
C	1.107397291389156	-2.861736931836067	0.007486353024570
C	-0.685835156041517	4.254407395748069	-0.047999479150224
C	2.437795505716274	-2.433008376793065	0.007553225678890
C	-4.251065729617023	0.688689855594608	-0.035692695754193
C	-1.108487082212999	2.871591734365544	-0.001470075830382
C	-2.866125559491756	1.111274227312668	-0.003199144564242
C	-4.250591668764654	-0.681476568604424	-0.030877141797987
C	-2.865603138584163	-1.103089260384689	0.003941847655646
C	-2.438920371277259	2.441891644012002	-0.005277559529072
C	4.251065729617028	0.688689855594608	-0.035692695754193
C	2.866125559491762	1.111274227312668	-0.003199144564242
C	4.250591668764650	-0.681476568604424	-0.030877141797987
C	2.865603138584158	-1.103089260384689	0.003941847655646
N	0.000000000000000	2.041842054603320	0.029067029430216
N	0.000000000000000	-2.032832070643810	0.024485544594906
N	-2.036384785279232	0.004455734291536	0.017325815456104
N	2.036384785279226	0.004455734291536	0.017325815456104
H	5.103110076401324	-1.357624608611026	-0.051197223241747
H	-5.103683065565273	1.364706465943690	-0.061102752326484
H	-5.103110076401332	-1.357624608611026	-0.051197223241747
H	-1.361013533293658	5.107308073077707	-0.081568070199502
H	1.361013533293662	5.107308073077707	-0.081568070199502
H	5.103683065565278	1.364706465943690	-0.061102752326484
H	-1.361262405727722	-5.098478427342194	-0.052561384759009
H	1.361262405727728	-5.098478427342194	-0.052561384759009
H	-3.211170189894045	3.213249697407476	-0.027987520556898
H	3.211170189894052	3.213249697407476	-0.027987520556898
H	-3.209696901097033	-3.204831283811629	-0.004845484025998
H	3.209696901097034	-3.204831283811629	-0.004845484025998
H	0.000000000000000	0.778681441159684	2.767940412985692
O	0.000000000000000	-0.054854554112294	2.265190446647024

Transition Metal: Mn; Functional Group: H; Adsorbate: OOH

Mn	-0.018567582902790	0.013699242687828	0.266422895910392
C	0.670604495427406	4.262531963274060	-0.066996417318446
C	1.092820833120014	2.877653413957180	-0.021444985545272
C	2.421849297960716	2.450915739025548	-0.013011188887664
C	-0.700950781491805	-4.238569522441480	-0.018971034860066
C	-1.123597253433562	-2.853054173936489	-0.000578295369584
C	-2.452633285932446	-2.425719134272427	-0.018157643891424
C	0.668584040796746	-4.238747298721632	-0.008652551146653
C	1.091400025623658	-2.853624924443093	0.017711237638176
C	-0.698927047047441	4.263103463633234	-0.071932978009553
C	2.420648644943736	-2.427484190730386	0.025175938523940
C	-4.260756800805538	0.698942260803542	-0.091419222004866
C	-1.122275090301311	2.878317746007790	-0.031963274091846
C	-2.879291142829103	1.120769183425946	-0.044812721119840
C	-4.261110211101167	-0.672968696773339	-0.084890167578830
C	-2.879799868038088	-1.094989097342463	-0.034248158160342
C	-2.451494230299534	2.451431002729240	-0.042889244986808
C	4.232185720260023	0.697162459105462	-0.021609244202878
C	2.850135998050672	1.120076897354338	0.000843027132592
C	4.231977730935804	-0.674928235092562	-0.009417859818413
C	2.849682169059166	-1.096782378696140	0.019495503873380
N	-0.015309734969510	2.047119649035980	-0.000649832610326
N	-0.016296671620380	-2.022183802634483	0.021703616794758
N	-2.048420961557948	0.012771149513196	-0.013795396450568
N	2.019358402568246	0.011972550195214	0.022855056561174
H	5.085164958961474	-1.350459696119167	-0.023668451959505
H	-5.113090104524769	1.374715658444772	-0.127502285776053
H	-5.113929323969501	-1.348475359668580	-0.113456995822368
H	-1.374943188776957	5.115347741392780	-0.106565502160308
H	1.347466393611486	5.114257595878082	-0.096814132789287
H	5.085438450378714	1.372146086459478	-0.048602736081790
H	-1.377403964529989	-5.090922499168837	-0.041132199217568
H	1.344917636259838	-5.091335020580253	-0.020923249070556
H	-3.223456387869771	3.222979225673960	-0.067167354607748
H	3.194136223784652	3.222211810727806	-0.030374807544830
H	-3.224894070960406	-3.197257499197409	-0.033100799179856
H	3.192626751992696	-3.199431643997695	0.023301952950144
H	-0.705404329075819	-0.007906855048342	3.933894126022214
O	0.152850148777336	0.019663709921554	2.248004901171028
O	-1.086295890474492	0.002471479617996	3.032030473684916

Transition Metal: Mn; Functional Group: NH2; Adsorbate: Clean

Mn	0.033526926437866	-0.025436544779520	-0.049104346744372
C	0.832473594583166	4.141981154886626	-0.518060349654949
C	1.205448966343430	2.753891402157442	-0.498903314790457
C	2.527509274266062	2.244033635079086	-0.625699378947296
C	-0.710338581552417	-4.194642738757690	-0.450261429394779
C	-1.114738599879562	-2.815753414489134	-0.411979245273820
C	-2.420765827063395	-2.319481637122163	-0.605768306036715
C	0.632802960993958	-4.240584251947970	-0.083071296600853
C	1.033846961779818	-2.890481623618143	0.211831775557678
C	-0.492942048287087	4.219050482687984	-0.097181810451417
C	2.326930295224258	-2.486359317829983	0.637676897716616
C	-4.151636499148609	0.725041542659410	0.394683189141576
C	-0.962919132911889	2.867931899760664	0.073779512419594
C	-2.768939143908501	1.155821720630792	0.301155805851992
C	-4.187168757450179	-0.616548357526373	0.054016980510492
C	-2.828419979661977	-1.023246109228008	-0.217283456362402
C	-2.310176682872996	2.491150526372656	0.312462813167500
C	4.244199509478724	0.571602385358862	0.198747725758416
C	2.903136013975254	0.952964590665642	-0.213364202417022
C	4.166744936290248	-0.721170791238912	0.688394983201028
C	2.797979893553608	-1.168260284179460	0.511749066444230
N	0.102367186670090	1.984803613896142	-0.135820350685261
N	-0.035006053725880	-2.023690191935216	-0.002738465994600
N	-1.962119215623112	0.051813979108630	0.003815409097748
N	2.025560808813724	-0.109985080305833	0.012705692776282
N	5.262172348326266	-1.503899308178113	1.203905020547496
N	-5.278646186179172	1.546784013881878	0.745669812263728
N	-5.346418031950266	-1.422140684856867	-0.006740165261628
N	-1.216721876695964	5.419290729244290	0.068814222416182
N	1.690235861678154	5.255405584890624	-0.840931952359806
N	5.403814177087241	1.351737804550044	0.133547038069408
N	-1.484010784856093	-5.334076841501865	-0.792614251395591
N	1.393720834595952	-5.433775198249762	-0.014682457923058
N	-3.254448491347887	3.536526106560446	0.508844402341592
N	3.566370731723572	3.124547131825334	-1.043651226582934
N	-3.407305276983791	-3.209375088058476	-1.126438687999539
N	3.210271365122630	-3.523447976293109	1.071976237412178
H	-2.436707802737896	-5.279605174247683	-0.423932941964548
H	-1.046461621815343	-6.181923717086553	-0.421137631148717
H	-3.002640211128714	-3.877995272404803	-1.783889293766070
H	-4.165038202944677	-2.707531979546204	-1.591903791888111
H	-5.499310927827105	1.520603139412052	1.746924789015812
H	-6.120015293619947	1.290632633609278	0.224117688585404
H	-1.861796575907295	5.383548993591024	0.860598524542716
H	1.224191916230880	5.918854825894262	-1.465943926332422
H	1.994217730542610	5.772505686718857	-0.008371252769962
H	3.194801887192288	4.050984340949798	-1.286436961745025
H	4.112974920638542	2.734970193706784	-1.813723542657868
H	5.201870794212068	2.351837422294052	0.045882595060622
H	6.071264402165220	1.146803049506202	0.878047991649386
H	6.103454617870186	-1.391645284433455	0.629554797143326
H	5.508650954879823	-1.241110671997120	2.164502335184360
H	4.148160766035614	-3.145124892408734	1.256635287529918
H	2.855455817767146	-3.996195311417225	1.907515093298140
H	2.384626305530010	-5.211126448471076	0.130237626900558
H	1.293377924863460	-5.992171681438093	-0.866765145891847
H	-5.171893000645786	-2.394315868453234	0.255655765870356
H	-6.099491837239633	-1.043647920279259	0.571714626136276
H	-4.212925492851785	3.165944748046836	0.521852197489368
H	-3.169061681966422	4.268262267480374	-0.200098987770755
H	-0.593838725208812	6.224519573834623	0.159627051771666

Transition Metal: Mn; Functional Group: NH2; Adsorbate: O

Mn	0.023387832749382	-0.023693122144284	0.313371009212144
C	0.787039719486000	4.119910235744786	-0.535302507978166
C	1.166788526920632	2.725972342924058	-0.486529468038679
C	2.486633319368442	2.219499802312932	-0.646081211656483
C	-0.692471785572753	-4.182718545615566	-0.460587097283398
C	-1.096262507215489	-2.795667101261511	-0.419812033260659
C	-2.382760423050005	-2.291340755111012	-0.694356630389674
C	0.623455860679744	-4.238946541041692	-0.029104205127076
C	1.012197866036870	-2.880556980284211	0.302181291990848
C	-0.501273854745218	4.204402090317602	-0.022648635818964
C	2.298099749666930	-2.474382797418031	0.737922252904360
C	-4.154628257129190	0.715624190820188	0.360937353350654
C	-0.955512440264009	2.853171935108398	0.214289689394080
C	-2.773341292924087	1.137393213286742	0.350539452263776
C	-4.184100839741552	-0.605321448103815	-0.072502086054544
C	-2.814276178148191	-0.994133948718655	-0.309982999422274
C	-2.299483017081837	2.471389853980946	0.483960745603310
C	4.229376251175680	0.564892848237908	0.176349542152684
C	2.882165212598164	0.931853741680370	-0.222242796746720
C	4.155774331432028	-0.718329825703272	0.704474284107240
C	2.788711179926060	-1.160783854674158	0.557094959130220
N	0.090093169341686	1.975507203661146	-0.040759738178441
N	-0.040190724056490	-2.020133174164886	0.050824497417304
N	-1.971922148275532	0.067583434952658	-0.016868162546692
N	2.024148434681486	-0.130923890980444	0.023552929294710
N	5.247775099540034	-1.487551620544693	1.244891989177834
N	-5.293684096339469	1.525427619123194	0.687461947379112
N	-5.347643988653253	-1.386572188872801	-0.235984750421355
N	-1.245965078508373	5.398561978519339	0.153920827210842
N	1.618693627654302	5.218693645829676	-0.964909628976596
N	5.391472281725777	1.337728920409978	0.067821309751782
N	-1.484902935803142	-5.294886029302099	-0.882244934651098
N	1.405566726377018	-5.415174583432481	0.043906282107020
N	-3.228376094326148	3.469923701274510	0.796276821173200
N	3.510098507857292	3.095916804488726	-1.089170032347351
N	-3.351461381479854	-3.152510163218857	-1.277323676574817
N	3.168531919187174	-3.490878003280443	1.213248386763100
H	-2.357959309788448	-5.351776497515903	-0.347276049132542
H	-0.982071160147903	-6.169054113781369	-0.708522576957364
H	-2.925504070312147	-3.944233576271074	-1.764050644625019
H	-3.977283483722978	-2.652962802286641	-1.910673038367051
H	-5.521099932811538	1.506435821579154	1.687241279138278
H	-6.125081148584732	1.244045620348046	0.162514337748942
H	-1.561449344564483	5.518845031717614	1.120655865154350
H	1.204170642288156	5.728521928437008	-1.750481350499992
H	1.796123574379816	5.892161731836966	-0.212189581572105
H	3.141230072015878	4.025588358093272	-1.324087690541212
H	4.068047396417998	2.702237530657460	-1.848146498879068
H	5.190302502322957	2.338810550646560	-0.008569199941798
H	6.074282207841870	1.135551990547390	0.799771301411472
H	6.090256288441608	-1.402621067669600	0.667914039515172
H	5.492801523907466	-1.189190603350877	2.195397021166116
H	4.105306718925844	-3.118582562722580	1.411022484295608
H	2.788013195693554	-3.980355253460864	2.025469365093456
H	2.388058173074078	-5.182021871364437	0.222793443151598
H	1.340365845953990	-5.975246558753531	-0.809526624860176
H	-5.165299430910782	-2.388808118227264	-0.150169553371412
H	-6.087588681043201	-1.109841911952490	0.412885702113044
H	-4.199247699214508	3.155472944876844	0.683443682750262
H	-3.041504249098413	4.364725718835480	0.340466071218440
H	-0.693499350399513	6.218538557370033	-0.108937544851516
O	0.007135287124650	0.038037541309778	1.995392215604528

Transition Metal: Mn; Functional Group: NH2; Adsorbate: OH

Mn	0.013988176292740	-0.023806281883921	0.350460497054744
C	0.792745628326770	4.151301050194734	-0.520784139038806
C	1.174826417246396	2.760680365985844	-0.437294140607314
C	2.496186032345954	2.243720652126530	-0.576548027317763
C	-0.707946626842759	-4.206034407442608	-0.460441379368760
C	-1.118546108385992	-2.823140178828393	-0.375611124878624
C	-2.409689662788178	-2.312339342319447	-0.620103901034796
C	0.625462561832784	-4.258962056043625	-0.081496998035632
C	1.012726842306460	-2.904484831649370	0.269236830964376
C	-0.525253270951133	4.234117805843836	-0.085104051482286
C	2.310149650572306	-2.499738101351735	0.676455451825160
C	-4.170310477203907	0.723291680676248	0.376260091759140
C	-0.979442576845408	2.883721147273196	0.156818021683002
C	-2.791917246516352	1.151448789693576	0.327618644965926
C	-4.198601017641977	-0.617598896501335	0.007849855824172
C	-2.831423631824631	-1.008669530955753	-0.239703474681338
C	-2.328647185482488	2.496136275605144	0.393239544706290
C	4.228373122199958	0.569560596716622	0.222522815440774
C	2.881439672066300	0.946889403586252	-0.168893041259700
C	4.158081970125462	-0.733586719207931	0.700208380747510
C	2.791707275632128	-1.175858989417030	0.537261093392102
N	0.090243989535686	2.014324789012182	-0.016160370558463
N	-0.060715624647973	-2.055048620086673	0.091371598307844
N	-1.990480098324092	0.067586196612556	-0.001804412441550
N	2.025842854563832	-0.127551444715802	0.041036546708674
N	5.258689371876306	-1.518054476435697	1.198836247937420
N	-5.312389179755506	1.538028808965778	0.672078445463218
N	-5.361356833719565	-1.411435852985218	-0.084110404371621
N	-1.281145757674661	5.427572186495028	0.026675059151026
N	1.640460022424100	5.251379741397834	-0.913596662381551
N	5.388639054546857	1.348983172532878	0.153504592729890
N	-1.506036517072310	-5.317937670201189	-0.867077578230610
N	1.415977154545974	-5.431204498608789	-0.060181417185198
N	-3.276125177500223	3.504854440332080	0.620721623749678
N	3.529619751780824	3.118508675486004	-1.006573858277214
N	-3.392922549139726	-3.168677944036933	-1.188734776440533
N	3.197294774533596	-3.528712098859003	1.096940667245832
H	-2.366038237331129	-5.380531640349908	-0.312393067222938
H	-0.995246362795164	-6.191059430777877	-0.711888015174598
H	-2.977376415898402	-3.963196253226286	-1.680382705951750
H	-4.016582300859362	-2.665113816960986	-1.821425076624209
H	-5.496651814580790	1.620062571771076	1.677374429257844
H	-6.157015506910213	1.184934774733284	0.216288972990936
H	-1.687903763886062	5.547657759532166	0.958593408467462
H	1.234394485304450	5.796172475815364	-1.679605989350293
H	1.832195681004664	5.894140100916117	-0.137658789286519
H	3.163321348890064	4.049437268592098	-1.241110667499477
H	4.081237303398148	2.728666691318078	-1.772491322900073
H	5.186234231469927	2.349782446660446	0.078214450601192
H	6.058248326935239	1.140647555350568	0.895457693804104
H	6.104078179180712	-1.372975350420706	0.638374515348156
H	5.488530933140659	-1.287274341838671	2.171653974107354
H	4.139895935521838	-3.159631101698029	1.272156171625136
H	2.846369704994716	-4.029396751762649	1.916497683002168
H	2.400434231288288	-5.193945420015442	0.104117824342758
H	1.336711207803122	-5.965246493452907	-0.929135603609843
H	-5.160704692061584	-2.411577541908684	-0.019157770880784
H	-6.060141750651615	-1.149952072173917	0.614771651405214
H	-4.240709838813752	3.174828883260722	0.500061938700774
H	-3.086846683772379	4.368674722185212	0.109826328641792
H	-0.707496664331785	6.247460159249838	-0.185739559916582
H	0.454572983363572	0.759280369495672	2.732826927306124
O	-0.022757159961348	0.021813002727966	2.313171990443442

Transition Metal: Mn; Functional Group: NH2; Adsorbate: OOH

Mn	0.010038596061370	-0.020307013935913	0.301437538610876
C	0.790810036363518	4.145846358741451	-0.532317215801573
C	1.170819383897126	2.753450221476326	-0.455751695825040
C	2.493777346437754	2.241701332988370	-0.585388843388344
C	-0.707379478602110	-4.201554122595518	-0.463561424682300
C	-1.119237005049062	-2.818415480360429	-0.383694063999904
C	-2.410855021812598	-2.313278584709636	-0.628911137118514
C	0.623455286796818	-4.254512893944259	-0.080324269482418
C	1.011149886710896	-2.899373055010223	0.268492243829500
C	-0.523661500553143	4.229101673199772	-0.090882397519149
C	2.305888385450602	-2.497808488308230	0.679096118279940
C	-4.167044863911713	0.723763427767428	0.367123274429150
C	-0.980261874231200	2.878337744457626	0.145338253427842
C	-2.791558083105926	1.151509413094460	0.317488388651946
C	-4.196774693715835	-0.617774157248434	-0.002337566101940
C	-2.832608566285369	-1.009414889478531	-0.250944383582961
C	-2.327961370877272	2.495076905467840	0.388100368629672
C	4.223782563474278	0.570270556169242	0.221098350061912
C	2.878704826806908	0.947919319434678	-0.171347701401089
C	4.151753177457594	-0.731439133721942	0.703787563735888
C	2.785753832155414	-1.172646978574850	0.544379399495974
N	0.084148139267630	2.006149354988986	-0.041124577080836
N	-0.061224838202829	-2.046457264530595	0.083241384704790
N	-1.989497410581681	0.066268467670722	-0.011303458701803
N	2.020815612362056	-0.123700315103235	0.046396364037062
N	5.252356121605968	-1.512877096257387	1.207382943527826
N	-5.306769766707225	1.535711799108052	0.675657574780220
N	-5.360132874935168	-1.410804009713925	-0.087428272058446
N	-1.278910138683063	5.421944869601084	0.030304451341394
N	1.641141363455598	5.246696676963538	-0.917024847944724
N	5.384856002031784	1.347933394657268	0.152293084470010
N	-1.506512637273389	-5.313497848664035	-0.870163593287199
N	1.413800518289332	-5.426792211800491	-0.052907843095760
N	-3.272817580417204	3.503891582227072	0.624525064305776
N	3.529606662059864	3.117510288081974	-1.008950515247886
N	-3.396050563725705	-3.172951331437108	-1.192315227871788
N	3.196297664324256	-3.527795835217518	1.094804859875732
H	-2.364296297681715	-5.374911175014931	-0.311367653820902
H	-0.995358798764862	-6.186431959201212	-0.714533065278612
H	-2.979772857365862	-3.965683910131077	-1.686599921424268
H	-4.021774909691834	-2.670410086526946	-1.824020292201585
H	-5.480365338004509	1.612955280361050	1.683252381791480
H	-6.155152981082077	1.182838317274960	0.227038801259546
H	-1.679089774819037	5.536107706685440	0.965896313696696
H	1.242232590980938	5.791885141502783	-1.686435618665808
H	1.824562579567784	5.888386543862944	-0.138326046198486
H	3.164197851801020	4.049100114527485	-1.242884123622954
H	4.082221645897846	2.728805952728088	-1.774842016936727
H	5.180977077150271	2.348782022870462	0.077131312424430
H	6.052371058588139	1.140091542447378	0.896431389802588
H	6.097509999184359	-1.370198553220835	0.645943720602990
H	5.482353590783098	-1.274117172733330	2.178235741322848
H	4.138344558503338	-3.156362467365216	1.268665590056418
H	2.850590339285670	-4.028475201984634	1.916765010460076
H	2.399140521379858	-5.189092047366204	0.106064520903172
H	1.330189973388970	-5.969157933794859	-0.916237370791329
H	-5.159217219307429	-2.410569378952271	-0.016026171006814
H	-6.055506377243487	-1.144220387788867	0.612867911751306
H	-4.238679660034608	3.175201920016072	0.510347771750244
H	-3.086545055596645	4.368137610061788	0.112808221143964
H	-0.705506633268719	6.242537235179776	-0.180307305600540
H	-0.689571220137804	-0.008120746519012	3.981044904520306
O	0.171500000955042	0.075876949490614	2.292636446380782
O	-1.075459554101649	-0.048580625597000	3.083387582498522

Transition Metal: Mn; Functional Group: OH; Adsorbate: Clean

H	9.363239999999999	16.813980000000001	8.219110000000001
H	7.982940000000000	15.232139999999999	7.118080000000000
H	12.401710000000000	5.371780000000000	6.477380000000000
H	14.036160000000001	6.768150000000000	7.417950000000000
H	10.130610000000001	4.876690000000000	8.022770000000000
H	11.957990000000001	17.130700000000001	7.573940000000000
H	6.741660000000000	7.986120000000000	8.486490000000000
H	17.108329999999999	11.970570000000000	8.345760000000000
H	16.079219999999999	8.634040000000001	7.679210000000000
H	15.246980000000001	14.050369999999999	8.511220000000000
H	5.919580000000000	13.365080000000001	7.425820000000000
H	4.878680000000000	10.047860000000000	8.157389999999999
C	10.327010000000000	15.228730000000001	7.597220000000000
C	9.909179999999999	13.854559999999999	7.595670000000000
C	8.589160000000000	13.418080000000000	7.461050000000000
C	11.658310000000000	6.801560000000000	7.587130000000000
C	12.082640000000000	8.174930000000000	7.608880000000000
C	13.412050000000001	8.604240000000001	7.548360000000000
C	10.320589999999999	6.763790000000000	7.909700000000000
C	9.888750000000000	8.138760000000000	8.038890000000000
C	11.682570000000000	15.264889999999999	7.832340000000000
C	8.563459999999999	8.570650000000001	8.217990000000000
C	15.205859999999999	11.668580000000000	8.188219999999999
C	12.113099999999999	13.892329999999999	7.982130000000000
C	13.846410000000001	12.117430000000001	8.134740000000001
C	15.219030000000000	10.313680000000000	7.919410000000000
C	13.850030000000000	9.922359999999999	7.746370000000000
C	13.431229999999999	13.464829999999999	8.203419999999999
C	6.778140000000000	11.699930000000000	7.762030000000000
C	8.151669999999999	12.098789999999999	7.658240000000000
C	6.784960000000000	10.351330000000001	8.061620000000000
C	8.147390000000000	9.911960000000001	8.094690000000000
Mn	11.000439999999999	11.016340000000000	7.856110000000000
O	9.488040000000000	16.340080000000000	7.373490000000000
O	7.576020000000000	14.338390000000000	7.178500000000000
O	12.493840000000001	5.678680000000000	7.400630000000000
O	14.432760000000000	7.667490000000000	7.365620000000000
O	9.536619999999999	5.652340000000000	8.055809999999999
O	12.480230000000001	16.375699999999998	7.908890000000000
O	7.636080000000000	7.587000000000000	8.461020000000000
O	16.289429999999999	12.491860000000001	8.440650000000000
O	16.361860000000000	9.556030000000000	7.861190000000000
O	14.354699999999999	14.450930000000000	8.454340000000000
O	5.635770000000000	12.452070000000001	7.646320000000000
O	5.694480000000000	9.528370000000001	8.283870000000000
N	11.014049999999999	13.030370000000000	7.825990000000000
N	10.981890000000000	8.997760000000000	7.855760000000000
N	13.010109999999999	11.028260000000000	7.880010000000000
N	8.991040000000000	11.004379999999999	7.860440000000000

Transition Metal: Mn; Functional Group: OH; Adsorbate: O

H	9.393170000000000	16.846129999999999	7.391180000000000
H	8.011830000000000	15.201560000000001	6.354750000000000
H	12.353619999999999	5.417270000000000	5.687850000000000
H	14.013199999999999	6.792190000000000	6.621820000000000
H	10.113740000000000	4.880200000000000	7.268190000000000
H	11.995469999999999	17.111580000000000	6.857640000000000
H	6.764460000000000	8.001110000000001	7.947780000000000
H	17.109480000000001	11.985429999999999	7.632910000000000
H	16.071750000000002	8.655130000000000	6.860580000000000
H	15.222580000000001	14.033220000000000	7.969390000000000
H	5.929450000000000	13.336130000000001	6.626140000000000
H	4.880250000000000	10.025150000000000	7.475050000000000
C	10.335150000000001	15.212289999999999	6.877190000000000
C	9.926580000000000	13.837660000000000	6.871860000000000
C	8.603920000000000	13.389300000000000	6.718820000000000
C	11.648410000000000	6.817330000000000	6.858700000000000
C	12.068600000000000	8.188980000000001	6.890090000000000
C	13.400440000000000	8.625810000000000	6.803110000000000
C	10.316680000000000	6.770220000000000	7.217320000000000
C	9.895130000000000	8.142670000000001	7.387110000000000
C	11.680410000000000	15.257800000000000	7.181770000000000
C	8.573810000000000	8.581960000000000	7.612850000000000
C	15.207730000000000	11.669280000000001	7.480180000000000
C	12.101129999999999	13.886740000000000	7.359600000000000
C	13.839549999999999	12.112560000000000	7.464810000000000
C	15.218600000000000	10.328930000000000	7.165110000000000
C	13.838979999999999	9.939890000000000	7.003630000000000
C	13.419850000000000	13.449320000000000	7.605190000000000
C	6.780400000000000	11.682040000000001	7.035910000000000
C	8.163750000000000	12.075910000000000	6.923590000000000
C	6.785360000000000	10.352620000000000	7.395240000000000
C	8.155419999999999	9.916470000000000	7.443200000000000
Mn	10.998559999999999	11.014540000000000	7.475540000000000
O	10.995240000000001	11.029310000000001	9.154460000000000
O	9.502860000000000	16.309809999999999	6.581660000000000
O	7.603540000000000	14.307490000000000	6.418580000000000
O	12.478009999999999	5.703110000000000	6.614180000000000
O	14.410259999999999	7.692680000000000	6.585300000000000
O	9.528870000000000	5.659770000000000	7.342940000000000
O	12.477190000000000	16.368590000000001	7.270880000000000
O	7.661980000000000	7.607520000000000	7.920390000000000
O	16.286349999999999	12.499779999999999	7.728730000000000
O	16.357109999999999	9.573840000000001	7.051990000000000
O	14.326050000000000	14.426890000000000	7.919510000000000
O	5.643180000000000	12.426600000000001	6.854740000000000
O	5.702200000000000	9.523790000000000	7.630850000000000
N	11.020940000000000	13.034250000000000	7.152420000000000
N	10.976640000000000	8.994070000000001	7.176640000000000
N	13.006430000000000	11.038670000000000	7.169790000000000
N	8.993910000000000	10.986730000000000	7.152810000000000

Transition Metal: Mn; Functional Group: OH; Adsorbate: OH

H	10.891830000000001	9.994380000000000	9.770180000000000
H	9.508760000000001	16.962930000000000	7.301990000000000
H	7.954880000000000	15.261620000000001	6.638750000000000
H	12.547760000000000	5.448410000000000	5.475260000000000
H	14.036479999999999	6.746970000000000	6.806050000000000
H	10.073890000000000	4.825260000000000	6.603310000000000
H	11.982600000000000	17.139030000000002	6.357050000000000
H	6.694980000000000	7.959710000000000	7.315350000000000
H	17.113160000000001	11.978330000000000	7.567550000000000
H	16.071210000000001	8.608140000000001	7.231030000000000
H	15.289960000000001	14.067159999999999	7.453240000000000
H	5.909210000000000	13.399260000000000	7.035680000000000
H	4.872110000000000	10.026280000000000	7.331720000000000
C	10.327980000000000	15.275119999999999	6.750650000000000
C	9.913930000000001	13.907650000000000	6.891040000000000
C	8.582570000000000	13.446479999999999	6.924400000000000
C	11.669840000000001	6.760170000000000	6.633200000000000
C	12.078690000000000	8.120020000000000	6.852540000000000
C	13.408490000000000	8.578790000000000	6.961930000000000
C	10.292280000000000	6.711600000000000	6.744400000000000
C	9.863429999999999	8.073729999999999	6.990750000000000
C	11.707720000000000	15.310060000000000	6.828770000000000
C	8.536370000000000	8.532500000000001	7.177800000000000
C	15.206329999999999	11.675100000000000	7.453450000000000
C	12.132569999999999	13.943199999999999	7.046020000000000
C	13.848940000000001	12.131220000000001	7.322960000000000
C	15.207720000000000	10.302339999999999	7.334550000000000
C	13.832269999999999	9.904660000000000	7.156790000000000
C	13.456930000000000	13.488049999999999	7.251990000000000
C	6.776520000000000	11.713419999999999	7.205550000000000
C	8.155530000000001	12.117830000000000	7.091460000000000
C	6.780800000000000	10.341020000000000	7.327860000000000
C	8.145379999999999	9.890610000000001	7.254470000000000
Mn	10.994109999999999	11.042190000000000	7.540010000000000
O	10.993530000000000	10.901550000000000	9.431050000000001
O	9.470789999999999	16.370439999999999	6.525570000000000
O	7.554760000000000	14.375540000000001	6.795650000000000
O	12.523610000000000	5.655200000000000	6.430140000000000
O	14.437130000000000	7.642150000000000	6.892660000000000
O	9.490280000000000	5.608990000000000	6.632930000000000
O	12.518900000000000	16.408799999999999	6.723050000000000
O	7.583850000000000	7.549590000000000	7.247440000000000
O	16.297219999999999	12.510460000000000	7.621670000000000
O	16.347169999999998	9.539970000000000	7.362540000000000
O	14.402550000000000	14.474030000000001	7.359040000000000
O	5.632960000000000	12.469200000000001	7.179000000000000
O	5.686200000000000	9.501590000000000	7.450030000000000
N	11.025520000000000	13.110650000000000	7.062370000000000
N	10.966229999999999	8.906549999999999	7.045590000000000
N	13.009530000000000	11.030720000000001	7.153280000000000
N	8.985070000000000	10.998840000000000	7.125410000000000

Transition Metal: Mn; Functional Group: OH; Adsorbate: OOH

H	9.4001300000000001	16.874680000000001	6.524660000000000
H	7.9931800000000000	15.229970000000000	5.530270000000000
H	12.3825800000000001	5.412160000000000	4.775030000000000
H	14.0170800000000000	6.786070000000000	5.775720000000000
H	10.093579999999999	4.865690000000000	6.258440000000000
H	11.9874800000000000	17.132909999999999	5.892670000000000
H	6.7258200000000000	7.984080000000000	6.875990000000000
H	17.109439999999999	11.990910000000000	6.667570000000000
H	16.0625100000000000	8.650910000000000	6.013560000000000
H	15.244809999999999	14.058780000000000	6.939660000000000
H	5.9249900000000000	13.363460000000000	5.778500000000000
H	4.8656700000000000	10.033310000000000	6.457320000000000
H	10.3637800000000000	10.761189999999999	10.228710000000000
C	10.3285800000000001	15.239830000000000	5.989520000000000
C	9.9156200000000001	13.866339999999999	6.014760000000000
C	8.5913400000000001	13.416230000000001	5.883010000000000
C	11.6438700000000000	6.805160000000000	5.934310000000000
C	12.063689999999999	8.176119999999999	6.004080000000000
C	13.3963800000000001	8.618750000000000	5.952700000000000
C	10.2978700000000000	6.756320000000000	6.235810000000000
C	9.872999999999999	8.127459999999999	6.413710000000000
C	11.6846400000000000	15.282730000000001	6.240980000000000
C	8.5471900000000001	8.567270000000001	6.611020000000000
C	15.204359999999999	11.680920000000000	6.559790000000000
C	12.1060000000000000	13.911670000000001	6.424730000000000
C	13.838789999999999	12.127459999999999	6.547230000000000
C	15.210129999999999	10.329240000000000	6.287450000000000
C	13.8312800000000000	9.935860000000000	6.151100000000000
C	13.428229999999999	13.473220000000000	6.643770000000000
C	6.7732300000000000	11.697020000000000	6.133320000000000
C	8.154389999999999	12.097220000000000	6.065360000000000
C	6.7722700000000000	10.350250000000001	6.429000000000000
C	8.1383500000000001	9.911400000000000	6.488920000000000
Mn	10.9873700000000000	11.020750000000000	6.562150000000000
O	9.4917200000000001	16.339070000000000	5.712390000000000
O	7.5844300000000000	14.337050000000000	5.603380000000000
O	12.4803500000000000	5.692360000000000	5.706250000000000
O	14.414429999999999	7.686550000000000	5.756300000000000
O	9.5060100000000000	5.644530000000000	6.317320000000000
O	12.4869200000000000	16.391850000000002	6.287810000000000
O	7.6207600000000000	7.585560000000000	6.850750000000000
O	16.290669999999999	12.510260000000001	6.773820000000000
O	16.3487000000000001	9.573600000000001	6.186410000000000
O	14.350289999999999	14.456830000000000	6.897280000000000
O	5.6368900000000000	12.445160000000000	5.968730000000000
O	5.6809800000000000	9.518950000000000	6.605720000000000
O	11.1847600000000001	11.005900000000000	8.539339999999999
O	9.9606900000000000	10.828450000000000	9.339410000000001
N	11.012499999999999	13.064460000000000	6.277910000000000
N	10.9656900000000000	8.974880000000001	6.270400000000000
N	13.0033200000000000	11.041639999999999	6.303010000000000
N	8.9803200000000001	10.999040000000001	6.275370000000000

Transition Metal: Ni; Functional Group: BH2; Adsorbate: Clean

N	10.764290000000001	12.981400000000001	7.263770000000000
N	10.937760000000001	9.014130000000000	7.287850000000000
N	12.813850000000000	11.090999999999999	7.347620000000000
N	8.940500000000000	10.976590000000000	7.362720000000000
Ni	10.865280000000000	11.021030000000000	7.319340000000000
C	10.153680000000000	15.258410000000000	7.043660000000000
C	9.686380000000000	13.864080000000000	7.151380000000000
C	8.351200000000000	13.423270000000000	7.232210000000000
C	11.577080000000000	6.736270000000000	7.106740000000000
C	12.031960000000000	8.140599999999999	7.157390000000000
C	13.342980000000001	8.603510000000000	7.199370000000000
C	10.193390000000001	6.781740000000000	7.301550000000000
C	9.848960000000000	8.185650000000001	7.379100000000000
C	11.545970000000001	15.178410000000000	7.163060000000000
C	8.498200000000001	8.561150000000000	7.503380000000000
C	15.094820000000000	11.714250000000000	7.540140000000000
C	11.882180000000000	13.790160000000000	7.277160000000000
C	13.696370000000000	12.175950000000000	7.460020000000000
C	15.019430000000000	10.327590000000001	7.399690000000000
C	13.624020000000000	9.982490000000000	7.309180000000000
C	13.250420000000000	13.495780000000000	7.387700000000000
C	6.692620000000000	11.666850000000000	7.454190000000000
C	8.083620000000000	12.063820000000000	7.344150000000000
C	6.681610000000000	10.282590000000001	7.536410000000000
C	8.096610000000000	9.902760000000001	7.473850000000000
B	9.429390000000000	16.550450000000001	6.620070000000000
B	6.967590000000000	14.233140000000001	7.302040000000000
B	12.280450000000000	5.441910000000000	6.665880000000000
B	14.712160000000001	7.777000000000000	7.242110000000000
B	9.103400000000001	5.638390000000000	7.343460000000000
B	12.823750000000000	16.099329999999998	7.149310000000000
B	7.461610000000000	7.494930000000000	7.639310000000000
B	16.391269999999999	12.427830000000000	7.973610000000000
B	15.949439999999999	9.059030000000000	7.388510000000000
B	14.095179999999999	14.856320000000000	7.318650000000000
B	5.750840000000000	12.920529999999999	7.456520000000000
B	5.529520000000000	9.216030000000000	7.653150000000000
H	8.372400000000001	16.551850000000002	6.051620000000000
H	9.993550000000001	17.600030000000000	6.797820000000000
H	6.235830000000000	13.816129999999999	8.345570000000000
H	6.797970000000000	15.414880000000000	7.287700000000000
H	11.712350000000001	4.397940000000000	6.873660000000000
H	13.315890000000000	5.419460000000000	6.059440000000000
H	14.860120000000000	6.593820000000000	7.213230000000000
H	15.596380000000000	8.265480000000000	6.357430000000000
H	9.016100000000000	4.938730000000000	8.325130000000000
H	8.673640000000001	5.189060000000000	6.307330000000000
H	13.714060000000000	15.600009999999999	6.268380000000000
H	12.905010000000001	17.289010000000001	7.055630000000000
H	6.243380000000000	7.703450000000000	7.714890000000000
H	7.692350000000000	6.278630000000000	7.736980000000000
H	16.390950000000000	13.433500000000000	8.629189999999999
H	17.444400000000002	11.902360000000000	7.717850000000000
H	15.475180000000000	8.170510000000000	8.278480000000000
H	17.141800000000000	8.990819999999999	7.455550000000000
H	13.623790000000000	15.763019999999999	8.185879999999999
H	15.281630000000000	14.986100000000000	7.347740000000000
H	4.558070000000000	12.981290000000000	7.545950000000000
H	6.083800000000000	13.738780000000000	6.425690000000000
H	4.919430000000000	8.885070000000001	6.663700000000000
H	5.007640000000000	9.010650000000000	8.723520000000001

Transition Metal: Ni; Functional Group: BH2; Adsorbate: O

Ni	10.865530000000000	11.022880000000001	7.462120000000000
C	10.146250000000000	15.318849999999999	6.766240000000000
C	9.670249999999999	13.920000000000000	6.899990000000000
C	8.335960000000000	13.436310000000001	6.936560000000000
C	11.585480000000000	6.680100000000000	6.834900000000000
C	12.043310000000000	8.090529999999999	6.904140000000000
C	13.351000000000001	8.594659999999999	6.919240000000000
C	10.191710000000000	6.726460000000000	6.975270000000000
C	9.841600000000000	8.137280000000001	7.054190000000000
C	11.543509999999999	15.230370000000001	6.854910000000000
C	8.482260000000000	8.540740000000000	7.119170000000000
C	15.140790000000001	11.725569999999999	7.084960000000000
C	11.877739999999999	13.836980000000001	6.985310000000000
C	13.734610000000000	12.194210000000000	7.067900000000000
C	15.053970000000000	10.332070000000000	6.988290000000000
C	13.651289999999999	9.985110000000001	6.972460000000000
C	13.254920000000000	13.516299999999999	7.028380000000000
C	6.656660000000000	11.665060000000000	7.034140000000000
C	8.054330000000000	12.065090000000000	6.988130000000000
C	6.638270000000000	10.275960000000000	7.092930000000000
C	8.060510000000001	9.888010000000000	7.075780000000000
B	9.421060000000001	16.617989999999999	6.361780000000000
B	6.943270000000000	14.237450000000001	6.968870000000000
B	12.293960000000000	5.377270000000000	6.426460000000000
B	14.728260000000001	7.775020000000000	6.929510000000000
B	9.099550000000001	5.585830000000000	6.970720000000000
B	12.832290000000000	16.136050000000001	6.785400000000000
B	7.437020000000000	7.474150000000000	7.205890000000000
B	16.464600000000001	12.437180000000000	7.435470000000000
B	15.976730000000000	9.055930000000000	6.975030000000000
B	14.098480000000000	14.878600000000000	6.916620000000000
B	5.717870000000000	12.923859999999999	7.030290000000000
B	5.478850000000000	9.216020000000000	7.170050000000000
H	8.347000000000000	16.629770000000001	5.826590000000000
H	9.993960000000000	17.664249999999999	6.529810000000000
H	6.164750000000000	13.792170000000000	7.965770000000000
H	6.775130000000000	15.419280000000001	6.976530000000000
H	11.717169999999999	4.337400000000000	6.631980000000000
H	13.346530000000000	5.342240000000000	5.851270000000000
H	14.874440000000000	6.591330000000000	6.930600000000000
H	15.572880000000000	8.232780000000000	5.987920000000000
H	8.960060000000000	4.897570000000000	7.954210000000000
H	8.708000000000000	5.134960000000000	5.920650000000000
H	13.681820000000000	15.618350000000000	5.875050000000000
H	12.928300000000000	17.323910000000001	6.681450000000000
H	6.219310000000000	7.689130000000000	7.236980000000000
H	7.669280000000000	6.257620000000000	7.291220000000000
H	16.505009999999999	13.457590000000000	8.066260000000000
H	17.500520000000002	11.899190000000001	7.139660000000000
H	15.536060000000001	8.202909999999999	7.916300000000000
H	17.170300000000001	8.977490000000000	6.994120000000000
H	13.662750000000001	15.793659999999999	7.794990000000000
H	15.285769999999999	15.002670000000000	6.902460000000000
H	4.522550000000000	12.991130000000000	7.066610000000000
H	6.100250000000000	13.766850000000000	6.038980000000000
H	4.895090000000000	8.886939999999999	6.165250000000000
H	4.938620000000000	8.994389999999999	8.227940000000000
O	10.892530000000001	11.004899999999999	9.178450000000000
N	10.747450000000001	13.059130000000000	7.019230000000000
N	10.941680000000000	8.938750000000001	7.015460000000000
N	12.867590000000000	11.105700000000001	7.005670000000000
N	8.890440000000000	10.966670000000001	7.002020000000000

Transition Metal: Ni; Functional Group: BH2; Adsorbate: OH

Ni	10.866840000000000	11.032340000000000	7.000380000000000
C	10.157090000000000	15.276450000000001	6.581360000000000
C	9.684659999999999	13.883950000000000	6.702430000000000
C	8.349430000000000	13.433890000000000	6.779020000000000
C	11.580209999999999	6.727970000000000	6.641080000000000
C	12.036659999999999	8.134440000000000	6.696580000000000
C	13.345160000000000	8.605790000000001	6.743920000000000
C	10.196980000000000	6.774010000000000	6.840610000000000
C	9.853450000000000	8.182110000000000	6.926250000000000
C	11.551140000000000	15.193440000000001	6.695350000000000
C	8.504110000000001	8.564240000000000	7.062950000000000
C	15.108660000000000	11.718280000000000	7.066400000000000
C	11.886870000000000	13.805940000000000	6.823410000000000
C	13.708530000000000	12.184990000000001	6.991580000000000
C	15.027410000000000	10.330990000000000	6.935530000000000
C	13.629080000000000	9.987610000000000	6.848550000000000
C	13.256750000000000	13.505250000000000	6.926630000000000
C	6.691640000000000	11.670940000000000	6.987930000000000
C	8.082020000000000	12.072590000000000	6.882260000000000
C	6.683710000000000	10.285670000000000	7.072660000000000
C	8.101620000000000	9.906960000000000	7.020180000000000
B	9.428610000000001	16.569009999999999	6.163820000000000
B	6.961370000000000	14.239560000000001	6.845490000000000
B	12.284129999999999	5.432910000000000	6.201310000000000
B	14.714040000000001	7.778230000000000	6.794070000000000
B	9.100149999999999	5.637240000000000	6.872650000000000
B	12.832020000000000	16.111129999999999	6.670400000000000
B	7.467740000000000	7.501430000000000	7.221900000000000
B	16.414010000000001	12.428400000000000	7.482210000000000
B	15.953490000000000	9.057510000000001	6.934080000000000
B	14.101620000000000	14.867260000000000	6.846540000000000
B	5.747790000000000	12.923880000000000	6.988070000000000
B	5.535010000000000	9.211470000000000	7.162730000000000
H	10.606240000000000	11.807570000000000	9.354920000000000
H	8.356180000000000	16.573879999999999	5.625780000000000
H	10.002219999999999	17.616479999999999	6.321200000000000
H	6.225980000000000	13.817909999999999	7.883340000000000
H	6.791110000000000	15.421080000000000	6.833680000000000
H	11.716170000000000	4.389990000000000	6.413630000000000
H	13.319400000000000	5.409850000000000	5.594930000000000
H	14.857609999999999	6.594220000000000	6.771620000000000
H	15.602399999999999	8.258490000000000	5.906860000000000
H	9.025240000000000	4.910680000000000	7.835320000000000
H	8.646129999999999	5.222650000000000	5.832030000000000
H	13.718370000000000	15.603960000000001	5.790910000000000
H	12.915319999999999	17.299650000000000	6.566640000000000
H	6.251480000000000	7.715700000000000	7.321380000000000
H	7.701490000000000	6.286140000000000	7.325660000000000
H	16.430850000000000	13.455730000000001	8.101699999999999
H	17.458420000000000	11.877300000000000	7.245780000000000
H	15.473480000000000	8.178150000000000	7.829610000000000
H	17.145309999999998	8.985210000000000	7.005910000000000
H	13.632650000000000	15.781020000000000	7.708080000000000
H	15.287770000000000	14.997010000000000	6.872040000000000
H	4.554850000000000	12.982820000000000	7.072490000000000
H	6.083270000000000	13.746960000000000	5.962010000000000
H	4.978130000000000	8.854600000000000	6.150960000000000
H	4.957560000000000	9.032539999999999	8.208750000000000
O	10.900430000000000	10.939120000000001	9.015340000000000
N	10.763350000000001	13.008940000000001	6.818930000000000
N	10.940980000000000	8.997400000000001	6.824050000000000
N	12.833980000000000	11.100000000000000	6.875940000000000
N	8.932390000000000	10.982559999999999	6.892130000000000

Transition Metal: Ni; Functional Group: BH2; Adsorbate: OOH

Ni	10.865530000000000	11.022880000000001	7.462120000000000
C	10.146250000000000	15.318849999999999	6.766240000000000
C	9.670249999999999	13.920000000000000	6.899990000000000
C	8.335960000000000	13.436310000000001	6.936560000000000
C	11.585480000000000	6.680100000000000	6.834900000000000
C	12.043310000000000	8.090529999999999	6.904140000000000
C	13.351000000000001	8.594659999999999	6.919240000000000
C	10.191710000000000	6.726460000000000	6.975270000000000
C	9.841600000000000	8.137280000000001	7.054190000000000
C	11.543509999999999	15.230370000000001	6.854910000000000
C	8.482260000000000	8.540740000000000	7.119170000000000
C	15.140790000000001	11.725569999999999	7.084960000000000
C	11.877739999999999	13.836980000000001	6.985310000000000
C	13.734610000000000	12.194210000000000	7.067900000000000
C	15.053970000000000	10.332070000000000	6.988290000000000
C	13.651289999999999	9.985110000000001	6.972460000000000
C	13.254920000000000	13.516299999999999	7.028380000000000
C	6.656660000000000	11.665060000000000	7.034140000000000
C	8.054330000000000	12.065090000000000	6.988130000000000
C	6.638270000000000	10.275960000000000	7.092930000000000
C	8.060510000000001	9.888010000000000	7.075780000000000
B	9.421060000000001	16.617989999999999	6.361780000000000
B	6.943270000000000	14.237450000000001	6.968870000000000
B	12.293960000000000	5.377270000000000	6.426460000000000
B	14.728260000000001	7.775020000000000	6.929510000000000
B	9.099550000000001	5.585830000000000	6.970720000000000
B	12.832290000000000	16.136050000000001	6.785400000000000
B	7.437020000000000	7.474150000000000	7.205890000000000
B	16.464600000000001	12.437180000000000	7.435470000000000
B	15.976730000000000	9.055930000000000	6.975030000000000
B	14.098480000000000	14.878600000000000	6.916620000000000
B	5.717870000000000	12.923859999999999	7.030290000000000
B	5.478850000000000	9.216020000000000	7.170050000000000
H	8.347000000000000	16.629770000000001	5.826590000000000
H	9.993960000000000	17.664249999999999	6.529810000000000
H	6.164750000000000	13.792170000000000	7.965770000000000
H	6.775130000000000	15.419280000000001	6.976530000000000
H	11.717169999999999	4.337400000000000	6.631980000000000
H	13.346530000000000	5.342240000000000	5.851270000000000
H	14.874440000000000	6.591330000000000	6.930600000000000
H	15.572880000000000	8.232780000000000	5.987920000000000
H	8.960060000000000	4.897570000000000	7.954210000000000
H	8.708000000000000	5.134960000000000	5.920650000000000
H	13.681820000000000	15.618350000000000	5.875050000000000
H	12.928300000000000	17.323910000000001	6.681450000000000
H	6.219310000000000	7.689130000000000	7.236980000000000
H	7.669280000000000	6.257620000000000	7.291220000000000
H	16.505009999999999	13.457590000000000	8.066260000000000
H	17.500520000000002	11.899190000000001	7.139660000000000
H	15.536060000000001	8.202909999999999	7.916300000000000
H	17.170300000000001	8.977490000000000	6.994120000000000
H	13.662750000000001	15.793659999999999	7.794990000000000
H	15.285769999999999	15.002670000000000	6.902460000000000
H	4.522550000000000	12.991130000000000	7.066610000000000
H	6.100250000000000	13.766850000000000	6.038980000000000
H	4.895090000000000	8.886939999999999	6.165250000000000
H	4.938620000000000	8.994389999999999	8.227940000000000
N	10.747450000000001	13.059130000000000	7.019230000000000
N	10.941680000000000	8.938750000000001	7.015460000000000
N	12.867590000000000	11.105700000000001	7.005670000000000
N	8.890440000000000	10.966670000000001	7.002020000000000
O	10.898591163074730	11.000863714367272	9.563744667409260
H	9.333487249574532	11.497100263723958	10.518444787151587
O	9.769351080747558	10.629512193694644	10.370218322097703

Transition Metal: Ni; Functional Group: CH3; Adsorbate: Clean

Ni	10.967400000000000	11.053390000000000	7.408660000000000
C	10.484570000000000	15.189880000000000	7.649520000000000
C	9.970319999999999	13.819860000000000	7.705230000000000
C	8.630770000000000	13.421390000000001	7.930980000000000
C	11.578070000000000	6.983970000000000	8.177680000000001
C	11.960089999999999	8.394250000000000	8.222340000000001
C	13.215470000000000	8.907560000000000	8.620920000000000
C	10.411560000000000	6.908550000000000	7.433140000000000
C	10.020759999999999	8.281800000000000	7.123000000000000
C	11.707649999999999	15.135439999999999	7.002580000000000
C	8.766100000000000	8.704969999999999	6.633360000000000
C	15.093310000000001	11.551670000000000	6.951480000000000
C	12.008419999999999	13.724930000000001	6.792550000000000
C	13.699180000000000	11.961220000000001	6.797350000000000
C	15.092960000000000	10.439390000000000	7.778390000000000
C	13.694100000000001	10.103210000000001	8.034260000000000
C	13.238429999999999	13.205880000000001	6.318250000000000
C	6.833490000000000	11.580679999999999	7.757970000000000
C	8.211069999999999	12.078690000000000	7.768090000000000
C	6.865000000000000	10.316720000000000	7.193970000000000
C	8.269380000000000	9.980840000000001	6.994920000000000
C	9.921700000000000	16.433740000000000	8.296609999999999
C	7.573380000000000	14.500000000000000	8.116350000000001
C	12.348250000000000	5.805000000000000	8.714969999999999
C	14.060330000000000	8.169219999999999	9.645080000000000
C	9.644539999999999	5.646970000000000	7.129890000000000
C	12.610200000000001	16.313479999999998	6.743300000000000
C	7.937650000000000	7.791890000000000	5.745300000000000
C	16.320570000000000	12.250570000000000	6.425750000000000
C	16.314609999999998	9.664520000000000	8.203320000000000
C	14.057919999999999	14.010339999999999	5.323630000000000
C	5.600090000000000	12.203840000000000	8.369490000000001
C	5.670090000000000	9.419969999999999	6.999870000000000
N	10.972030000000000	12.951390000000000	7.281120000000000
N	10.986030000000000	9.153010000000000	7.595280000000000
N	12.878030000000001	11.043320000000000	7.431360000000000
N	9.061719999999999	11.042740000000000	7.393440000000000
H	9.349390000000000	16.204070000000002	9.204770000000000
H	10.740399999999999	17.104939999999999	8.597260000000000
H	9.264430000000001	17.019079999999999	7.629310000000000
H	6.632330000000000	14.215199999999999	7.639720000000000
H	7.356920000000000	14.715940000000000	9.176869999999999
H	7.877600000000000	15.436730000000001	7.644400000000000
H	12.369560000000000	5.773150000000000	9.816670000000000
H	11.905139999999999	4.860070000000000	8.373300000000000
H	13.394399999999999	5.806640000000000	8.372260000000001
H	14.679880000000001	8.879180000000000	10.206770000000001
H	13.413990000000000	7.665600000000000	10.374810000000000
H	14.735130000000000	7.406210000000000	9.223839999999999
H	9.633590000000000	5.400410000000000	6.055450000000000
H	10.081780000000000	4.787000000000000	7.654420000000000
H	8.595260000000000	5.717090000000000	7.454960000000000
H	12.241490000000001	17.208359999999999	7.262970000000000
H	13.640540000000000	16.135590000000001	7.087070000000000
H	12.666760000000000	16.572939999999999	5.673200000000000
H	8.595760000000000	7.169290000000000	5.126090000000000
H	7.257020000000000	7.113730000000000	6.284830000000000
H	7.326110000000000	8.389930000000000	5.057800000000000
H	16.353919999999999	13.308520000000000	6.729460000000000
H	17.234639999999999	11.781620000000000	6.813920000000000
H	16.386019999999998	12.228830000000000	5.325690000000000
H	16.528099999999998	9.756860000000000	9.281100000000000
H	16.215199999999999	8.590630000000001	7.984910000000000
H	17.206340000000001	10.015670000000000	7.667220000000000
H	14.828230000000000	14.656169999999999	5.775270000000000
H	14.568090000000000	13.336710000000000	4.623090000000000

H	13.400539999999999	14.653130000000001	4.725220000000000
H	4.903530000000000	11.418049999999999	8.697050000000001
H	5.837460000000000	12.806710000000001	9.255540000000000
H	5.040570000000000	12.849570000000000	7.669840000000000
H	5.806780000000000	8.431350000000000	7.465310000000000
H	4.770190000000000	9.867960000000000	7.442610000000000
H	5.443190000000000	9.246680000000000	5.935330000000000

Transition Metal: Ni; Functional Group: CH3; Adsorbate: O

Ni	10.977940000000000	11.004849999999999	6.832900000000000
C	10.445449999999999	15.240349999999999	7.582600000000000
C	9.939030000000000	13.867550000000000	7.504930000000000
C	8.583290000000000	13.456280000000000	7.614620000000000
C	11.596700000000000	6.902560000000000	8.096830000000001
C	11.994059999999999	8.314510000000000	8.064920000000001
C	13.271160000000000	8.833900000000000	8.405849999999999
C	10.348470000000001	6.823330000000000	7.497820000000000
C	9.946520000000000	8.194559999999999	7.183740000000000
C	11.752860000000000	15.214600000000001	7.121770000000000
C	8.656630000000000	8.622109999999999	6.777320000000000
C	15.200110000000000	11.619009999999999	7.006990000000000
C	12.076250000000000	13.815890000000000	6.861340000000000
C	13.807200000000000	12.040150000000001	6.853150000000000
C	15.176019999999999	10.413300000000000	7.692110000000000
C	13.765580000000000	10.058040000000000	7.877070000000000
C	13.347000000000000	13.318989999999999	6.453810000000000
C	6.773470000000000	11.618350000000000	7.699550000000000
C	8.151680000000001	12.103560000000000	7.574590000000000
C	6.780530000000000	10.283420000000000	7.326040000000000
C	8.174010000000001	9.926489999999999	7.076680000000000
C	9.785410000000001	16.446100000000001	8.208580000000000
C	7.514640000000000	14.542610000000000	7.576230000000000
C	12.398270000000000	5.717550000000000	8.574540000000001
C	14.137560000000001	8.067790000000000	9.394330000000000
C	9.538250000000000	5.563040000000000	7.333130000000000
C	12.687880000000000	16.395710000000001	7.081020000000000
C	7.757160000000000	7.670220000000000	6.005050000000000
C	16.444970000000001	12.370780000000000	6.611350000000000
C	16.395150000000001	9.600840000000000	8.051399999999999
C	14.217810000000000	14.201140000000001	5.573920000000000
C	5.578650000000000	12.331300000000001	8.287739999999999
C	5.587310000000000	9.363519999999999	7.350860000000000
N	10.989220000000000	13.026790000000000	7.169960000000000
N	10.965999999999999	9.059469999999999	7.522430000000000
N	12.974790000000000	11.061299999999999	7.360350000000000
N	8.977020000000000	11.025720000000000	7.295290000000000
O	11.008870000000000	10.839800000000000	5.119000000000000
H	9.093420000000000	16.165080000000000	9.013280000000000
H	10.543770000000000	17.107270000000000	8.654480000000000
H	9.219150000000001	17.058969999999999	7.485310000000000
H	6.625410000000000	14.191060000000000	7.043810000000000
H	7.191140000000000	14.881280000000000	8.574780000000001
H	7.874110000000000	15.420249999999999	7.030480000000000
H	12.464940000000000	5.660440000000000	9.673940000000000
H	11.947150000000001	4.777670000000000	8.229590000000000
H	13.427790000000000	5.735520000000000	8.188310000000000
H	14.769450000000001	8.763960000000001	9.958769999999999
H	13.504940000000000	7.550660000000000	10.125999999999999
H	14.801349999999999	7.312970000000000	8.942170000000001
H	9.419390000000000	5.268350000000000	6.277470000000000
H	10.009910000000000	4.719760000000000	7.854700000000000
H	8.527020000000000	5.670320000000000	7.753670000000000
H	12.291079999999999	17.230989999999998	7.675030000000000
H	13.683109999999999	16.152170000000002	7.481240000000000
H	12.834110000000001	16.779789999999998	6.057190000000000
H	8.363230000000000	7.027370000000000	5.353830000000000
H	7.133630000000000	7.010740000000000	6.630000000000000
H	7.082830000000000	8.239060000000000	5.352780000000000
H	16.450080000000000	13.395400000000000	7.013700000000000
H	17.344580000000001	11.874590000000000	6.998620000000000
H	16.561640000000001	12.452660000000000	5.518340000000000
H	16.635069999999999	9.639200000000001	9.127599999999999
H	16.274950000000000	8.541119999999999	7.784170000000000
H	17.279869999999999	9.965210000000001	7.511710000000000
H	14.970160000000000	14.795190000000000	6.117100000000000

H	14.755660000000001	13.585129999999999	4.841560000000000
H	13.593600000000000	14.900160000000000	5.004520000000000
H	4.894910000000000	11.608160000000000	8.756309999999999
H	5.869970000000000	13.046820000000000	9.067740000000001
H	4.987420000000000	12.884670000000000	7.537310000000000
H	5.804170000000000	8.414190000000000	7.863310000000000
H	4.740980000000000	9.831350000000000	7.872580000000000
H	5.231950000000000	9.111730000000000	6.337620000000000

Transition Metal: Ni; Functional Group: CH3; Adsorbate: OH

Ni	10.976360000000000	11.052560000000000	7.241740000000000
C	10.504670000000000	15.196500000000000	7.670250000000000
C	9.982350000000000	13.829300000000000	7.707300000000000
C	8.642049999999999	13.426420000000000	7.932850000000000
C	11.565790000000000	6.994130000000000	8.186220000000000
C	11.957620000000000	8.403820000000000	8.215120000000001
C	13.211140000000000	8.921410000000000	8.618399999999999
C	10.406180000000001	6.916680000000000	7.428900000000000
C	10.027580000000000	8.288029999999999	7.097450000000000
C	11.728899999999999	15.144690000000001	7.020660000000000
C	8.779180000000000	8.718380000000000	6.595390000000000
C	15.108420000000001	11.571300000000001	6.970480000000000
C	12.021839999999999	13.737959999999999	6.785350000000000
C	13.715220000000000	11.973940000000001	6.794250000000000
C	15.100870000000000	10.460240000000001	7.801410000000000
C	13.698560000000001	10.117509999999999	8.036550000000000
C	13.248710000000001	13.212610000000000	6.303430000000000
C	6.844800000000000	11.577800000000000	7.775460000000000
C	8.219010000000001	12.083760000000000	7.768080000000000
C	6.874160000000000	10.315530000000001	7.202240000000000
C	8.274800000000001	9.987940000000000	6.975480000000000
C	9.944559999999999	16.434930000000001	8.330650000000000
C	7.585740000000000	14.503640000000001	8.130070000000000
C	12.320840000000000	5.818000000000000	8.751150000000001
C	14.047590000000000	8.185860000000000	9.650910000000000
C	9.631930000000001	5.659280000000000	7.128400000000000
C	12.639989999999999	16.319630000000000	6.776320000000000
C	7.959590000000000	7.817420000000000	5.690680000000000
C	16.336819999999999	12.273709999999999	6.453540000000000
C	16.319360000000000	9.691179999999999	8.245310000000000
C	14.062160000000000	14.011170000000000	5.302470000000000
C	5.617560000000000	12.193550000000000	8.406910000000000
C	5.684080000000000	9.409480000000000	7.020810000000000
N	10.983400000000000	12.970630000000000	7.267080000000000
N	10.990320000000001	9.150539999999999	7.571330000000000
N	12.898009999999999	11.058410000000000	7.423130000000000
N	9.060400000000000	11.048249999999999	7.376910000000000
O	11.022650000000001	10.871890000000000	5.204590000000000
H	10.354640000000000	11.504260000000000	4.874440000000000
H	9.369400000000001	16.196130000000000	9.234460000000000
H	10.763970000000000	17.100919999999999	8.639600000000000
H	9.290310000000000	17.028269999999999	7.667670000000000
H	6.640500000000000	14.219189999999999	7.660910000000000
H	7.378590000000000	14.716040000000000	9.193300000000001
H	7.886460000000000	15.442259999999999	7.658610000000000
H	12.329090000000001	5.805720000000000	9.853330000000000
H	11.873250000000001	4.871290000000000	8.420820000000001
H	13.370320000000000	5.806290000000000	8.419240000000000
H	14.664800000000000	8.897069999999999	10.213530000000000
H	13.395289999999999	7.686010000000000	10.377860000000000
H	14.723030000000000	7.420000000000000	9.235440000000001
H	9.627630000000000	5.413010000000000	6.054150000000000
H	10.058130000000000	4.797250000000000	7.658290000000000
H	8.580909999999999	5.739970000000000	7.445560000000000
H	12.283149999999999	17.210400000000000	7.311140000000000
H	13.670170000000001	16.125520000000002	7.111170000000000
H	12.692430000000000	16.592390000000002	5.709320000000000
H	8.627120000000000	7.213710000000000	5.062680000000000
H	7.283130000000000	7.124690000000000	6.217320000000000
H	7.346330000000000	8.425490000000000	5.013500000000000
H	16.364170000000001	13.331820000000000	6.757040000000000
H	17.250550000000000	11.808040000000000	6.845340000000000
H	16.403359999999999	12.250830000000001	5.354050000000000
H	16.516919999999999	9.788430000000000	9.325710000000001
H	16.225739999999998	8.616429999999999	8.028409999999999
H	17.216840000000001	10.043730000000000	7.719840000000000

H	14.843120000000001	14.649450000000000	5.747360000000000
H	14.555980000000000	13.330560000000000	4.596930000000000
H	13.402340000000001	14.659509999999999	4.712850000000000
H	4.928940000000000	11.403969999999999	8.741740000000000
H	5.866420000000000	12.795170000000001	9.290620000000001
H	5.045750000000000	12.838609999999999	7.716460000000000
H	5.841180000000000	8.418530000000001	7.474470000000000
H	4.786490000000000	9.843389999999999	7.481690000000000
H	5.444570000000000	9.244149999999999	5.957890000000000

Transition Metal: Ni; Functional Group: CH3; Adsorbate: OOH

C	10.977940000000000	11.004849999999999	6.832900000000000
C	10.445449999999999	15.240349999999999	7.582600000000000
C	9.939030000000000	13.867550000000000	7.504930000000000
C	8.583290000000000	13.456280000000000	7.614620000000000
C	11.596700000000000	6.902560000000000	8.096830000000001
C	11.994059999999999	8.314510000000000	8.064920000000001
C	13.271160000000000	8.833900000000000	8.405849999999999
C	10.348470000000001	6.823330000000000	7.497820000000000
C	9.946520000000000	8.194559999999999	7.183740000000000
C	11.752860000000000	15.214600000000001	7.121770000000000
C	8.656630000000000	8.622109999999999	6.777320000000000
C	15.200110000000000	11.619009999999999	7.006990000000000
C	12.076250000000000	13.815890000000000	6.861340000000000
C	13.807200000000000	12.040150000000001	6.853150000000000
C	15.176019999999999	10.413300000000000	7.692110000000000
C	13.765580000000000	10.058040000000000	7.877070000000000
C	13.347000000000000	13.318989999999999	6.453810000000000
C	6.773470000000000	11.618350000000000	7.699550000000000
C	8.151680000000001	12.103560000000000	7.574590000000000
C	6.780530000000000	10.283420000000000	7.326040000000000
C	8.174010000000001	9.926489999999999	7.076680000000000
C	9.785410000000001	16.446100000000001	8.208580000000000
C	7.514640000000000	14.542610000000000	7.576230000000000
C	12.398270000000000	5.717550000000000	8.574540000000001
C	14.137560000000001	8.067790000000000	9.394330000000000
C	9.538250000000000	5.563040000000000	7.333130000000000
C	12.687880000000000	16.395710000000001	7.081020000000000
C	7.757160000000000	7.670220000000000	6.005050000000000
C	16.444970000000001	12.370780000000000	6.611350000000000
C	16.395150000000001	9.600840000000000	8.051399999999999
C	14.217810000000000	14.201140000000001	5.573920000000000
C	5.578650000000000	12.331300000000001	8.287739999999999
C	5.587310000000000	9.363519999999999	7.350860000000000
N	10.989220000000000	13.026790000000000	7.169960000000000
N	10.965999999999999	9.059469999999999	7.522430000000000
N	12.974790000000000	11.061299999999999	7.360350000000000
N	8.977020000000000	11.025720000000000	7.295290000000000
H	9.093420000000000	16.165080000000000	9.013280000000000
H	10.543770000000000	17.107270000000000	8.654480000000000
H	9.219150000000001	17.058969999999999	7.485310000000000
H	6.625410000000000	14.191060000000000	7.043810000000000
H	7.191140000000000	14.881280000000000	8.574780000000001
H	7.874110000000000	15.420249999999999	7.030480000000000
H	12.464940000000000	5.660440000000000	9.673940000000000
H	11.947150000000001	4.777670000000000	8.229590000000000
H	13.427790000000000	5.735520000000000	8.188310000000000
H	14.769450000000001	8.763960000000001	9.958769999999999
H	13.504940000000000	7.550660000000000	10.125999999999999
H	14.801349999999999	7.312970000000000	8.942170000000001
H	9.419390000000000	5.268350000000000	6.277470000000000
H	10.009910000000000	4.719760000000000	7.854700000000000
H	8.527020000000000	5.670320000000000	7.753670000000000
H	12.291079999999999	17.230989999999998	7.675030000000000
H	13.683109999999999	16.152170000000002	7.481240000000000
H	12.834110000000001	16.779789999999998	6.057190000000000
H	8.363230000000000	7.027370000000000	5.353830000000000
H	7.133630000000000	7.010740000000000	6.630000000000000
H	7.082830000000000	8.239060000000000	5.352780000000000
H	16.450080000000000	13.395400000000000	7.013700000000000
H	17.344580000000001	11.874590000000000	6.998620000000000
H	16.561640000000001	12.452660000000000	5.518340000000000
H	16.635069999999999	9.639200000000001	9.127599999999999
H	16.274950000000000	8.541119999999999	7.784170000000000
H	17.279869999999999	9.965210000000001	7.511710000000000
H	14.970160000000000	14.795190000000000	6.117100000000000
H	14.755660000000001	13.585129999999999	4.841560000000000

H	13.593600000000000	14.900160000000000	5.004520000000000
H	4.894910000000000	11.608160000000000	8.756309999999999
H	5.869970000000000	13.046820000000000	9.067740000000001
H	4.987420000000000	12.884670000000000	7.537310000000000
H	5.804170000000000	8.414190000000000	7.863310000000000
H	4.740980000000000	9.831350000000000	7.872580000000000
H	5.231950000000000	9.111730000000000	6.337620000000000
O	11.015693096943659	10.803390295811479	4.740917043267457
H	9.742165450991216	9.674670933949566	3.897487598227776
O	9.834287892964372	10.651673130719761	3.937954704814478

Transition Metal: Ni; Functional Group: F; Adsorbate: Clean

Ni	0.000000000000000	-0.000121742969490	0.002638688430130
C	0.682483872257452	4.225334935720426	-0.007891403185397
C	1.101840445133540	2.845306539356926	-0.005381265883512
C	2.423175846513780	2.422906118700956	-0.000597137437580
C	-0.682470844846200	-4.225413631569033	-0.007294178605012
C	-1.101884204525852	-2.845365373632099	-0.002398825672832
C	-2.423339369841763	-2.423038828200134	-0.000497853363318
C	0.682470844846200	-4.225413631569033	-0.007294178605012
C	1.101884204525850	-2.845365373632099	-0.002398825672832
C	-0.682483872257450	4.225334935720426	-0.007891403185397
C	2.423339369841762	-2.423038828200134	-0.000497853363318
C	-4.226180972644455	0.682589536468134	0.004887930191230
C	-1.101840445133536	2.845306539356926	-0.005381265883512
C	-2.846017835815427	1.101770335928360	0.005003496804508
C	-4.226344008989965	-0.682372692154857	0.004622703837400
C	-2.846193095875236	-1.101780269840798	0.004804743091032
C	-2.423175846513775	2.422906118700956	-0.000597137437580
C	4.226180972644462	0.682589536468134	0.004887930191230
C	2.846017835815430	1.101770335928360	0.005003496804508
C	4.226344008989962	-0.682372692154857	0.004622703837400
C	2.846193095875234	-1.101780269840798	0.004804743091032
N	0.000000000000000	1.994252621346674	-0.004731785138128
N	0.000000000000000	-1.994397356617206	0.000011115054486
N	-1.995121511242942	-0.000069182012568	0.005759927450422
N	1.995121511242940	-0.000069182012568	0.005759927450422
F	5.306772237171694	-1.482371809882153	0.003078457037164
F	-5.306368776947579	1.482956189785264	0.003378689184674
F	-5.306772237171698	-1.482371809882153	0.003078457037164
F	-1.482818196466837	5.305505610927280	-0.005969127385718
F	1.482818196466842	5.305505610927280	-0.005969127385718
F	5.306368776947582	1.482956189785264	0.003378689184674
F	-1.482757045765130	-5.305614313583975	-0.008706459744662
F	1.482757045765128	-5.305614313583975	-0.008706459744662
F	-3.385480995609370	3.385552161432204	-0.000747329289538
F	3.385480995609370	3.385552161432204	-0.000747329289538
F	-3.385633984378213	-3.385552088323823	-0.004166376202368
F	3.385633984378216	-3.385552088323823	-0.004166376202368

Transition Metal: Ni; Functional Group: F; Adsorbate: O

Ni	0.000000000000000	-0.001280508984387	0.435456257184944
C	0.685684198276196	4.267020930293440	-0.013567743705732
C	1.108526135380126	2.885587733726282	-0.013577739083158
C	2.432529436118270	2.431674210629224	-0.007850795198152
C	-0.685697264034445	-4.268635992293381	-0.014299649881345
C	-1.108596331466330	-2.887241466426900	-0.015190495281680
C	-2.432617635643584	-2.433297361745907	-0.009210461434858
C	0.685697264034444	-4.268635992293381	-0.014299649881345
C	1.108596331466338	-2.887241466426900	-0.015190495281680
C	-0.685684198276199	4.267020930293440	-0.013567743705732
C	2.432617635643592	-2.433297361745907	-0.009210461434858
C	-4.268145726575870	0.684927358909994	-0.006982472598150
C	-1.108526135380117	2.885587733726282	-0.013577739083158
C	-2.886718573401062	1.107744507528788	-0.009878834178036
C	-4.268168065916667	-0.686474876176227	-0.007455584479702
C	-2.886763047370049	-1.109343438887024	-0.010639054946296
C	-2.432529436118262	2.431674210629224	-0.007850795198152
C	4.268145726575874	0.684927358909994	-0.006982472598150
C	2.886718573401064	1.107744507528788	-0.009878834178036
C	4.268168065916650	-0.686474876176227	-0.007455584479702
C	2.886763047370046	-1.109343438887024	-0.010639054946296
N	0.000000000000000	2.055239819767264	-0.025097216895924
N	0.000000000000000	-2.056976316418918	-0.027282906753317
N	-2.056554641970997	-0.000810674152694	-0.022731198560706
N	2.056554641970998	-0.000810674152694	-0.022731198560706
F	5.354980628107312	-1.478012175995591	-0.012235464578300
F	-5.354903296449333	1.476559688724626	-0.011282945757937
F	-5.354980628107313	-1.478012175995591	-0.012235464578300
F	-1.477233957152329	5.353855676289976	-0.018952408693306
F	1.477233957152338	5.353855676289976	-0.018952408693306
F	5.354903296449334	1.476559688724626	-0.011282945757937
F	-1.477210301468336	-5.355489542798439	-0.018627978780515
F	1.477210301468348	-5.355489542798439	-0.018627978780515
F	-3.394965986592304	3.394294648182218	0.000833633347576
F	3.394965986592304	3.394294648182218	0.000833633347576
F	-3.395089777130107	-3.395888048061998	-0.000310311490698
F	3.395089777130102	-3.395888048061998	-0.000310311490698
O	0.000000000000000	-0.003545349856523	2.169712877065736

Transition Metal: Ni; Functional Group: F; Adsorbate: OH

Ni	0.000000000000000	-0.002596833680808	0.249246955160302
C	0.685865374568358	4.293850439107364	-0.006294519865442
C	1.105059847298980	2.910494116282176	-0.004080293777762
C	2.424783491135010	2.437684289477994	-0.007915109775210
C	-0.685346858601058	-4.291321242761159	-0.008479434975811
C	-1.102890727605875	-2.906155341365555	-0.019629729578262
C	-2.421868250388254	-2.433311137583058	-0.008389345619008
C	0.685346858601060	-4.291321242761159	-0.008479434975811
C	1.102890727605878	-2.906155341365555	-0.019629729578262
C	-0.685865374568348	4.293850439107364	-0.006294519865442
C	2.421868250388256	-2.433311137583058	-0.008389345619008
C	-4.254499568419121	0.686382744442492	0.008965594102902
C	-1.105059847298975	2.910494116282176	-0.004080293777762
C	-2.872738849769785	1.109929694719808	-0.013799194061118
C	-4.253107490728587	-0.683611777808345	0.011905684679036
C	-2.870427222543274	-1.104893856337206	-0.010921561420012
C	-2.424783491135003	2.437684289477994	-0.007915109775210
C	4.254499568419110	0.686382744442492	0.008965594102902
C	2.872738849769786	1.109929694719808	-0.013799194061118
C	4.253107490728598	-0.683611777808345	0.011905684679036
C	2.870427222543264	-1.104893856337206	-0.010921561420012
N	0.000000000000000	2.078218363756594	-0.006286855324712
N	0.000000000000000	-2.075705594171314	-0.036204983624094
N	-2.035990553696493	0.002511771799668	-0.050032045273493
N	2.035990553696482	0.002511771799668	-0.050032045273493
F	5.341241124756833	-1.474692251596668	0.014813784486006
F	-5.343885776618549	1.476284434952062	0.011083335539666
F	-5.341241124756831	-1.474692251596668	0.014813784486006
F	-1.479398298781664	5.380447951126632	-0.010679828888453
F	1.479398298781658	5.380447951126632	-0.010679828888453
F	5.343885776618528	1.476284434952062	0.011083335539666
F	-1.480414963211292	-5.376654287353841	-0.001774708529531
F	1.480414963211282	-5.376654287353841	-0.001774708529531
F	-3.394004484480796	3.391043380902878	0.003467616061610
F	3.394004484480808	3.391043380902878	0.003467616061610
F	-3.391913216713146	-3.384644045393202	0.013156785718524
F	3.391913216713142	-3.384644045393202	0.013156785718524
H	0.000000000000000	0.867553531758136	2.443816828804916
O	0.000000000000000	-0.057039232886396	2.126263997335716

Transition Metal: Ni; Functional Group: F; Adsorbate: OOH

Ni	-0.009880891798624	0.013993942621902	0.322044197822674
C	0.673593173319782	4.274735000755272	-0.032960880181098
C	1.096743439751878	2.893624874242994	-0.035654733908606
C	2.423089599965602	2.441466053636462	-0.005568787060662
C	-0.698737419674536	-4.248632968523955	-0.032967962198236
C	-1.123378275990913	-2.868010096228954	-0.041778495611042
C	-2.449382635801907	-2.414821706382494	-0.023798036201694
C	0.672837121745210	-4.248017947132617	-0.029151961104664
C	1.096099849692288	-2.867021434878229	-0.034734906859844
C	-0.698084509071595	4.275470479728479	-0.035386302370286
C	2.422282486293232	-2.415063269143502	-0.005434807840058
C	-4.296157303245780	0.699033652605104	-0.021754254800335
C	-1.123229866958713	2.895143017945024	-0.040805819811844
C	-2.912563478822172	1.120484582984634	-0.012498418080018
C	-4.295712747074196	-0.671608676730028	-0.023224522598696
C	-2.912108708679678	-1.092537758211854	-0.014402845472878
C	-2.449340600882678	2.442453995951964	-0.020791438331492
C	4.2711101069067550	0.698115324596212	0.007076509525924
C	2.887803076474358	1.120315590240260	0.015815990192896
C	4.270308905249620	-0.672772366278288	0.006213007753812
C	2.887069285706740	-1.094081286017207	0.015273082592142
N	-0.013764638819920	2.063175639708074	-0.054861682747283
N	-0.013872695374382	-2.036126728123065	-0.055985768856736
N	-2.083110353672865	0.014186176013642	-0.007783907590106
N	2.058537747918604	0.013364184081120	0.024079906222290
F	5.357691697485122	-1.466170853468235	-0.011966659989586
F	-5.384932576871279	1.490695407079690	-0.037870013826290
F	-5.383295337142940	-1.465115479825410	-0.040434994514008
F	-1.485909202671863	5.366603024067640	-0.031855226438320
F	1.463481010327614	5.364665535643443	-0.025781908493272
F	5.359890032354619	1.4897448299999836	-0.010237821218141
F	-1.486814620868625	-5.339725588032609	-0.026381546663434
F	1.462141180959580	-5.338216902597599	-0.016891175415724
F	-3.408285914513026	3.410602023629972	-0.005716940773886
F	3.382016020586348	3.409900986438724	0.001714773679456
F	-3.408732523190380	-3.382823045144626	-0.013531728646138
F	3.380866686540434	-3.383762742734909	0.000097037958904
H	-0.719227522926900	0.016221144405070	3.887441077056266
O	0.135621594463186	0.014030677355468	2.219772396138536
O	-1.068925200859901	0.012538818564810	2.966911091916474

Transition Metal: Ni; Functional Group: H; Adsorbate: Clean

Ni	0.000000000000000	-0.000085706898826	0.009226498456724
C	0.683301931926464	4.214322143484416	-0.011161327503718
C	1.099268078040668	2.830001403467386	-0.002151854053730
C	2.426827606050124	2.426612881970268	0.001654556454946
C	-0.683299874907888	-4.214285199524861	-0.009117368606617
C	-1.099316013605218	-2.830070051955587	0.001415203000734
C	-2.426937530459249	-2.426800194007615	0.003545652403596
C	0.683299874907894	-4.214285199524861	-0.009117368606617
C	1.099316013605218	-2.830070051955587	0.001415203000734
C	-0.683301931926465	4.214322143484416	-0.011161327503718
C	2.426937530459254	-2.426800194007615	0.003545652403596
C	-4.214884585894797	0.683468041357518	0.003104483369144
C	-1.099268078040669	2.830001403467386	-0.002151854053730
C	-2.830517359776380	1.099227766941928	0.007530374635506
C	-4.215088203204363	-0.683204652144560	0.003320191877514
C	-2.830841109453271	-1.099238894034759	0.008191265803328
C	-2.426827606050121	2.426612881970268	0.001654556454946
C	4.214884585894792	0.683468041357518	0.003104483369144
C	2.830517359776370	1.099227766941928	0.007530374635506
C	4.215088203204360	-0.683204652144560	0.003320191877514
C	2.830841109453264	-1.099238894034759	0.008191265803328
N	0.000000000000000	1.980451371098934	0.002023192290830
N	0.000000000000000	-1.980475590363177	0.006479377857136
N	-1.981007726807444	-0.000173316245148	0.011064401318226
N	1.981007726807446	-0.000173316245148	0.011064401318226
H	5.062341392365158	-1.366422762246128	-0.001749166792369
H	-5.061618259980280	1.367221018962158	-0.002562173963927
H	-5.062341392365163	-1.366422762246128	-0.001749166792369
H	-1.367032332392199	5.061090977585135	-0.015636397447857
H	1.367032332392196	5.061090977585135	-0.015636397447857
H	5.061618259980288	1.367221018962158	-0.002562173963927
H	-1.366906663612887	-5.061205254590737	-0.015976802218731
H	1.366906663612884	-5.061205254590737	-0.015976802218731
H	-3.198200131623349	3.198141515668060	-0.002009748710026
H	3.198200131623342	3.198141515668060	-0.002009748710026
H	-3.198253400628154	-3.198420461605831	-0.001480823868622
H	3.198253400628160	-3.198420461605831	-0.001480823868622

Transition Metal: Ni; Functional Group: H; Adsorbate: O

Ni	0.000000000000000	-0.000715513800898	0.467180270833938
C	0.685279428454930	4.255343774197994	-0.033102404850794
C	1.105875361107054	2.867838041571970	0.005234416876852
C	2.436324806077708	2.435335990072122	0.009830891907084
C	-0.685275611713021	-4.257153179591562	-0.032857181609110
C	-1.105873924724769	-2.869618602417461	0.006188492853260
C	-2.436279535893426	-2.437032115900433	0.009821698344268
C	0.685275611713026	-4.257153179591562	-0.032857181609110
C	1.105873924724772	-2.869618602417461	0.006188492853260
C	-0.685279428454933	4.255343774197994	-0.033102404850794
C	2.436279535893426	-2.437032115900433	0.009821698344268
C	-4.256760210764680	0.684315028010058	-0.022941404986632
C	-1.105875361107064	2.867838041571970	0.005234416876852
C	-2.869030484636180	1.104988073647098	0.009745734375338
C	-4.256633837734391	-0.686295958328941	-0.023086127949068
C	-2.868927431603581	-1.106768116528158	0.009649928405520
C	-2.436324806077710	2.435335990072122	0.009830891907084
C	4.256760210764684	0.684315028010058	-0.022941404986632
C	2.869030484636180	1.104988073647098	0.009745734375338
C	4.256633837734380	-0.686295958328941	-0.023086127949068
C	2.868927431603578	-1.106768116528158	0.009649928405520
N	0.000000000000000	2.039668018277412	0.019028925132408
N	0.000000000000000	-2.041493297906879	0.020857305105814
N	-2.040815375710139	-0.000847452857270	0.021021657286746
N	2.040815375710124	-0.000847452857270	0.021021657286746
H	5.109895425885976	-1.361780926462330	-0.050032046849822
H	-5.110353139830048	1.359338437100138	-0.049194873974784
H	-5.109895425885973	-1.361780926462330	-0.050032046849822
H	-1.360542330084705	5.108560777396174	-0.063595312934673
H	1.360542330084700	5.108560777396174	-0.063595312934673
H	5.110353139830042	1.359338437100138	-0.049194873974784
H	-1.360584131977443	-5.110280063712285	-0.064247456442889
H	1.360584131977436	-5.110280063712285	-0.064247456442889
H	-3.208479798320393	3.207695305300184	0.000473732178112
H	3.208479798320396	3.207695305300184	0.000473732178112
H	-3.208459869595231	-3.209394514073679	0.000226101308526
H	3.208459869595230	-3.209394514073679	0.000226101308526
O	0.000000000000000	0.000431798583350	2.195531811051428

Transition Metal: Ni; Functional Group: H; Adsorbate: OH

Ni	0.000000000000000	0.002550597613574	0.141905882667026
C	0.683958951042138	4.220929591557688	-0.017625220732970
C	1.102664319105798	2.837886074057390	0.001678059278510
C	2.430980116279362	2.430243830010490	0.002326647672406
C	-0.683428549972330	-4.218309749568467	-0.013296397550167
C	-1.100342432403252	-2.833072767988675	0.000642110804010
C	-2.428363277644216	-2.426066794798334	0.008779249773360
C	0.683428549972340	-4.218309749568467	-0.013296397550167
C	1.100342432403252	-2.833072767988675	0.000642110804010
C	-0.683958951042147	4.220929591557688	-0.017625220732970
C	2.428363277644206	-2.426066794798334	0.008779249773360
C	-4.223523248935983	0.684516369402986	-0.006867629275064
C	-1.102664319105799	2.837886074057390	0.001678059278510
C	-2.838661121137783	1.102457800261892	-0.004907363939126
C	-4.222201329664092	-0.682435563978785	-0.003381837061244
C	-2.836618846958316	-1.098452934686506	0.000176223313552
C	-2.430980116279351	2.430243830010490	0.002326647672406
C	4.223523248935986	0.684516369402986	-0.006867629275064
C	2.838661121137788	1.102457800261892	-0.004907363939126
C	4.222201329664096	-0.682435563978785	-0.003381837061244
C	2.836618846958312	-1.098452934686506	0.000176223313552
N	0.000000000000000	1.996300579091152	0.010161581338074
N	0.000000000000000	-1.993938296253713	-0.002366459835024
N	-1.997947941790173	0.002504734098140	-0.014210369768229
N	1.997947941790170	0.002504734098140	-0.014210369768229
H	5.068728468935882	-1.366248320147992	-0.004725158670414
H	-5.071473291181894	1.366291516058280	-0.011301515992674
H	-5.068728468935875	-1.366248320147992	-0.004725158670414
H	-1.366300588202201	5.068549252263782	-0.033388302496789
H	1.366300588202204	5.068549252263782	-0.033388302496789
H	5.071473291181898	1.366291516058280	-0.011301515992674
H	-1.366675463292953	-5.065006284831352	-0.024865151038433
H	1.366675463292960	-5.065006284831352	-0.024865151038433
H	-3.201686885711638	3.202292488498228	0.004423201038372
H	3.201686885711636	3.202292488498228	0.004423201038372
H	-3.199314738410127	-3.197850650674155	0.017602028589576
H	3.199314738410128	-3.197850650674155	0.017602028589576
H	0.000000000000000	0.871699962284546	2.488462133989586
O	0.000000000000000	-0.055950021804495	2.179349713950358

Transition Metal: Ni; Functional Group: H; Adsorbate: OOH

Ni	-0.001955979150336	-0.001792584886623	0.073872161938522
C	0.682399011520894	4.217237051969819	-0.015646161775717
C	1.098163647997676	2.832514205634952	-0.008944209930320
C	2.426279542990626	2.426884670043798	-0.004010590950590
C	-0.685397352885218	-4.217634681265057	-0.016983667889445
C	-1.102199003841378	-2.832774778623328	-0.013537266860842
C	-2.430110142040920	-2.427770184280391	-0.010462798993702
C	0.681107430733412	-4.217177373696831	-0.015141410922190
C	1.097304142169980	-2.832141197492358	-0.010051944462158
C	-0.684686727997242	4.218544425705806	-0.017136115897728
C	2.425414260423098	-2.427545704879222	-0.003653849390948
C	-4.221970510044002	0.683128306570432	-0.016055283279236
C	-1.102377997866103	2.834182253996480	-0.012015321264206
C	-2.837499993122837	1.100249174742946	-0.014185720902873
C	-4.221090468459787	-0.684103599705242	-0.016194876674902
C	-2.836675884148057	-1.100042498735167	-0.014062319754904
C	-2.430936701711197	2.428585774576958	-0.009163170188450
C	4.217993415428718	0.682767358308000	-0.007592477462740
C	2.833004159481126	1.099277785693558	-0.006068025476050
C	4.217778400379744	-0.684026018037436	-0.007184199618841
C	2.832737492940606	-1.100198834744262	-0.005414195250966
N	-0.002568299121176	1.989653574685666	-0.012662312458818
N	-0.002653081932682	-1.989338313977992	-0.016720759009510
N	-1.993521518884300	0.000022316051538	-0.016842377448540
N	1.990119686695912	-0.000514414705538	-0.010175857336606
H	5.064487913867484	-1.367619677688907	-0.008124083299030
H	-5.069373827839676	1.365970164544524	-0.019910552241569
H	-5.067660257188816	-1.367852530387925	-0.018776756410318
H	-1.367071640423273	5.066238901013785	-0.025535936674487
H	1.366554588424334	5.063507970602767	-0.021868777833721
H	5.064886572931721	1.366176938404326	-0.009275055896410
H	-1.368617507924913	-5.064612963771545	-0.021409680269606
H	1.365135221070522	-5.063558574634188	-0.017794919662890
H	-3.201999165183775	3.200428780507538	-0.008370150302404
H	3.197236455350616	3.198680672947092	0.000061471901700
H	-3.201023634610131	-3.199625886012107	-0.005474218310960
H	3.196060798981026	-3.199750920188947	0.002525060865206
H	-1.327557351122980	0.690011029561964	3.237649726840940
O	0.182079645731156	-0.000214598336406	2.335341583478874
O	-0.978795341619723	-0.220346019512320	3.093685039075896

Transition Metal: Ni; Functional Group: NH2; Adsorbate: Clean

Ni	0.007865240494938	-0.013437712946015	0.016470442335992
C	0.767547487854910	4.012758006078780	-0.822255557598940
C	1.162560952353868	2.632802673689450	-0.652798617540419
C	2.483383768936882	2.129698958663940	-0.752073752245366
C	-0.660517264394404	-4.056903412320432	-0.744053200161872
C	-1.110080115449932	-2.692739783344383	-0.568231629295688
C	-2.419788582476144	-2.207532093282985	-0.740344565759585
C	0.581633744877322	-4.154769443245545	-0.133337384560047
C	0.918841961692736	-2.825207047703195	0.339751526947122
C	-0.478293008042211	4.148143552072910	-0.223771481139963
C	2.165011753417750	-2.448206930219758	0.886555693112538
C	-4.048809117832555	0.720781761124642	0.679982388779830
C	-0.898986799586655	2.827347510541882	0.182308500464114
C	-2.675417126221813	1.147094580248504	0.528470287903380
C	-4.135786032646976	-0.563545312041626	0.161040208720988
C	-2.799468390680381	-0.935005825942007	-0.250116021611223
C	-2.200386139673025	2.476268521148094	0.629524552151848
C	4.143469304948112	0.542596171028994	0.332428828116266
C	2.832698424473204	0.885593014287880	-0.190744628181875
C	4.013421466541736	-0.689825962991421	0.955712955018240
C	2.654747744513828	-1.135121470226771	0.731603135567898
N	0.118999944558518	1.919794608470646	-0.072511158032615
N	-0.109030053221236	-1.945817172809580	0.046158246794228
N	-1.918749349744385	0.102254674538130	0.011084202750720
N	1.936210427982596	-0.137219909103798	0.081756887834256
N	5.052507071662410	-1.438115809104193	1.616985141962228
N	-5.139223567664651	1.516029513937324	1.168733940240528
N	-5.308007307231939	-1.337406886753264	0.066356776446996
N	-1.243675983576459	5.349361612102612	-0.109060578910274
N	1.573256736330818	5.057024488613910	-1.400949417702655
N	5.318620203212512	1.299792696047242	0.236113138190620
N	-1.411080414415547	-5.124279015905188	-1.356951872991658
N	1.357604943966088	-5.316678118688252	-0.010162650209172
N	-3.062147442729866	3.476766364331560	1.086561529005728
N	3.532050747335332	2.959742601837476	-1.226806944333532
N	-3.437970246332608	-3.061284147424395	-1.233931171633806
N	3.001671133241158	-3.469508241782400	1.410275208361862
H	-1.329333751612033	-5.990850089229090	-0.815700692698417
H	-1.086077568106059	-5.326582053903820	-2.308740477672270
H	-3.063969943411834	-3.981928309687717	-1.492647201430366
H	-3.979522611610843	-2.643587849123364	-1.992282167396205
H	-5.244674746681152	1.462658590582616	2.187534471955672
H	-6.025034084444691	1.230341517904616	0.743187437265906
H	-1.224702937382588	5.728664345528944	0.843492425318074
H	1.314408051508752	5.244819755498888	-2.375214150198708
H	1.482049703300126	5.936669415577746	-0.883228016390838
H	3.188554861487854	3.884939649505992	-1.506231821904812
H	4.088476156593222	2.522034538797252	-1.962653934120478
H	5.129344477612934	2.280365805626964	0.008830288084916
H	5.927753151898361	1.202534366804198	1.049725854218414
H	5.940790664703504	-1.365790370813393	1.111318818364822
H	5.216763254628122	-1.107649312106233	2.574018306160610
H	3.912496947351472	-3.092887392160677	1.699574763427910
H	2.558397628000474	-3.994829640337656	2.166062998559662
H	2.335149574310138	-5.103868316322668	0.211564385513582
H	1.273765636235420	-5.940027004586039	-0.814525256636450
H	-5.094037176996265	-2.327174433303835	-0.088774948206314
H	-5.920774261886146	-1.218334479685105	0.875900240691600
H	-4.047297330457143	3.189631180984778	1.067163895183562
H	-2.890204969520966	4.384998026429488	0.649522865209470
H	-0.886748701114787	6.073700562069124	-0.737526258036031

Transition Metal: Ni; Functional Group: NH2; Adsorbate: O

Ni	0.004217572506634	-0.004166767102284	0.557937756144358
C	0.799447334567294	4.107654152867654	-0.683660651232252
C	1.186136868417194	2.729820041500748	-0.468244886324239
C	2.521186239955708	2.227325177699366	-0.506718467022658
C	-0.692141034251602	-4.135500223373377	-0.649002213527858
C	-1.136478634197587	-2.786707559872767	-0.363754564915425
C	-2.468171497561944	-2.304392208379685	-0.450809826332868
C	0.633381600723530	-4.220015284198306	-0.243170032768933
C	1.000065584456240	-2.900692744678118	0.239354615822408
C	-0.524562856357775	4.221164804483422	-0.277710664107190
C	2.307083127274308	-2.519994291361300	0.653290926237190
C	-4.177955701059496	0.768245897136072	0.525103032798604
C	-0.972108320463690	2.891094610336814	0.071063430080132
C	-2.801746460138411	1.183819024250674	0.358009104729978
C	-4.226304485637367	-0.590906051119763	0.241778658594258
C	-2.871429416434250	-0.991092814552566	-0.080769415570618
C	-2.323733689969604	2.525246828210196	0.360507410313682
C	4.233524698132150	0.568315769201392	0.396866499366196
C	2.903464142023988	0.934559502348652	-0.065526696586982
C	4.154910226596115	-0.754866935835437	0.813377801049408
C	2.800703782926902	-1.194261668782222	0.557882817968594
N	0.087696199787018	2.009871152399626	-0.032435205712666
N	-0.078945495564881	-2.049300723295964	0.138447846916576
N	-2.021366559033709	0.092527707647582	0.026479054360636
N	2.051254970207048	-0.145920480697772	0.051978609293086
N	5.222431906407840	-1.550086518041649	1.370553785262408
N	-5.297852152141536	1.608197763958592	0.843374979729324
N	-5.389440175512654	-1.387828407388749	0.264071752437600
N	-1.304407931318124	5.414706043654988	-0.286236569903892
N	1.643567728346826	5.173168708432208	-1.170229831857487
N	5.387531470164609	1.364964751301700	0.421281446127856
N	-1.480359110747539	-5.196136886442789	-1.230715774850179
N	1.440135922735052	-5.366005861828018	-0.308777047151562
N	-3.242908599728693	3.542948769431076	0.598650786031240
N	3.560484306791824	3.111536296431038	-0.856798343098632
N	-3.481675738175976	-3.205301108334183	-0.822988256742907
N	3.194664114971246	-3.550959035454014	1.018667112494376
H	-1.375490620668401	-6.068981982898043	-0.703662707062808
H	-1.206741523078836	-5.390014078203579	-2.200519084743256
H	-3.111604766389750	-4.115649631429006	-1.125043766995219
H	-4.172660461732944	-2.818233889471362	-1.465117755183698
H	-5.427275590898512	1.734263742108542	1.852922974384218
H	-6.168431625856046	1.238291642494790	0.453820042171240
H	-1.517581541900434	5.741393312842936	0.662133071123964
H	1.393223937591120	5.455284457529982	-2.123363619190275
H	1.588904004849112	6.006544541404768	-0.575861209751778
H	3.217687087051184	4.031607079054882	-1.157152151503716
H	4.254776589909122	2.711980614864682	-1.487410942974655
H	5.181060421959648	2.366061500574916	0.439867252197590
H	6.040635031831406	1.098676048731738	1.159749936386724
H	6.092567108926332	-1.436644268764425	0.841037522255270
H	5.419890338687614	-1.297239548657750	2.345233916930916
H	4.113330979912206	-3.191910443237372	1.307042772183620
H	2.803462438742910	-4.219929962286798	1.681766980715912
H	2.439333156518344	-5.149764038050897	-0.285159358425183
H	1.202120277318680	-5.980733133033475	-1.088548064585940
H	-5.174382959056524	-2.381077065865110	0.377676403961162
H	-6.049373655734176	-1.084262584988448	0.983854612204630
H	-4.220574894572382	3.239345212487264	0.5288871666063460
H	-3.031485454853811	4.421526370799308	0.122278809018270
H	-0.812431588763296	6.169422690695287	-0.772080494176485
O	0.021001512390084	-0.001460701692121	2.302195312055038

Transition Metal: Ni; Functional Group: NH2; Adsorbate: OH

Ni	0.022710526986086	-0.007004870164760	0.296300900233826
C	0.786172806061848	4.007149436622278	-0.962288511342038
C	1.209779507422416	2.721207390154520	-0.461202833944501
C	2.542483216833910	2.290026625584592	-0.222672187613501
C	-0.696586411359458	-4.000478402299873	-1.057782768495244
C	-1.140013222564509	-2.711776383611273	-0.568810920111041
C	-2.477219829190719	-2.254997034338018	-0.452195836233539
C	0.652279655331540	-4.102608591052556	-0.742778008466971
C	1.015776073001224	-2.857930186118104	-0.091231173780462
C	-0.568818910683916	4.122281040439556	-0.668080741321120
C	2.295969809301512	-2.530143120050635	0.427795421687044
C	-4.029122009940094	0.748735447357840	0.917977782325828
C	-0.964932453118170	2.871654063789366	-0.065235500777190
C	-2.707596608349053	1.187673227174176	0.536923944387018
C	-4.105010717974103	-0.604608824119641	0.613957589823006
C	-2.818648119674126	-0.976335074401334	0.065577062591742
C	-2.269897619577620	2.532581025897610	0.421478267525578
C	4.099497339388686	0.602398181084684	0.892858927317818
C	2.859017719944232	0.995351260628990	0.256290025257814
C	4.014499925785108	-0.764621348141588	1.117266128447234
C	2.733166226518606	-1.193709614649887	0.605005106580286
N	0.109200555503324	2.021477510549794	0.016433160576100
N	-0.074449668659504	-2.017608947316550	-0.030589432668084
N	-1.965802926259126	0.115732735900334	0.062598122708168
N	2.020057740642140	-0.106119844388136	0.126220561878536
N	5.011661378656246	-1.609496769337490	1.723894275743552
N	-5.084843267779931	1.578685283712210	1.419704214913718
N	-5.238150138434669	-1.428869207630854	0.796492327607560
N	-1.438434425523297	5.245621623253732	-0.914446616452970
N	1.617349567095626	4.980781199087542	-1.597137505949981
N	5.201438911999120	1.422904527690990	1.204921227285640
N	-1.517008476304081	-4.993206988220642	-1.707622717998579
N	1.482268898918140	-5.209267692482255	-0.998272103565370
N	-3.126076571428513	3.559358035059140	0.750442044500484
N	3.581885356843636	3.223126554118580	-0.337440314507226
N	-3.516102394923017	-3.141359758535565	-0.759991236039525
N	3.200923635155930	-3.576354415846769	0.655822494030648
H	-1.309010357618028	-5.933980786525087	-1.359333252979905
H	-1.380009565586271	-5.004725956463812	-2.724391725644054
H	-3.188165366204526	-4.006483891356179	-1.205711388636644
H	-4.324745489783313	-2.720454186108302	-1.215082029339804
H	-5.004729157248459	1.756053668435226	2.426489154649090
H	-6.004151813594010	1.168566710458442	1.239885749387334
H	-0.988991932247330	6.137917226092732	-0.694721615557498
H	2.004086481964892	4.624388648745950	-2.477171524760621
H	1.082406415163620	5.823649344587212	-1.823712725476582
H	3.304228156732196	4.140385383725142	-0.688124942214245
H	4.457394105484062	2.874863697383734	-0.722917282622092
H	4.935962092637237	2.394832450221038	1.373483425183230
H	5.740774769526120	1.060458785329296	1.993617713053312
H	5.958872297125684	-1.343998387066897	1.440177528820280
H	4.970967929710788	-1.580499890783436	2.748551572128152
H	4.069487041901882	-3.259617812810099	1.103742952380096
H	2.794513506903380	-4.399734539218429	1.099501400756596
H	2.475018135350858	-4.967501173098645	-1.016362959898316
H	1.213924954284102	-5.719910496297814	-1.841260213150669
H	-4.989377637638469	-2.419437603142018	0.843787014692680
H	-5.767150333120441	-1.168286539647937	1.632121104598520
H	-4.114679735190354	3.313873813489202	0.835669039214246
H	-2.878028303733192	4.476220788970878	0.373083076966662
H	-1.762710812994463	5.286596353943802	-1.886335758347890
H	0.121491541099660	0.885364829108966	2.554108683925000
O	0.005456138309154	-0.043943075913218	2.278682458718232

Transition Metal: Ni; Functional Group: NH2; Adsorbate: OOH

Ni	0.023340352161876	-0.005330973796596	0.243460047429888
C	0.778579488257236	3.983228671449266	-0.979151374535594
C	1.205965256157096	2.698272223188300	-0.478625880819017
C	2.540374469902992	2.280472398775924	-0.242182751463996
C	-0.698781699801192	-3.977160885059412	-1.059357042901748
C	-1.144546042477216	-2.690887647756213	-0.568209456455385
C	-2.480760941737412	-2.242992775722353	-0.454700446791968
C	0.645338550695088	-4.085071777316426	-0.732756184627704
C	1.009161784417592	-2.845283041090742	-0.073134716215357
C	-0.570396559586342	4.103285143154670	-0.668012207140581
C	2.288688372654046	-2.529098623661817	0.443121660483734
C	-4.018206541779749	0.750677455404958	0.941824748278830
C	-0.963574744673373	2.857250298564150	-0.054549916981735
C	-2.694881349499092	1.190042047644234	0.566834241232188
C	-4.099140436167959	-0.597751086239995	0.620628214586870
C	-2.815460663172470	-0.968849030540969	0.069100048571340
C	-2.260372195291612	2.533613331334222	0.449277234186930
C	4.094093531490482	0.601534401472322	0.880969986587268
C	2.855703456575360	0.990719554394124	0.239338472751654
C	4.004704601122206	-0.762007492124301	1.120903900692496
C	2.723904365628464	-1.193713555917689	0.612389504438154
N	0.109310137433678	2.000064068116872	0.015346263622164
N	-0.080464861309700	-1.998799259094444	-0.015160176444894
N	-1.955290963998920	0.118607220524648	0.080921653210530
N	2.013101681489538	-0.109565470686000	0.119072048142218
N	4.998385746638868	-1.603642219270569	1.735244964400474
N	-5.081139966787307	1.578868421981564	1.429035114660134
N	-5.234888820600780	-1.418395147380117	0.792215602892984
N	-1.441623817407020	5.225007098958710	-0.914033073974128
N	1.601964711222802	4.955482415052646	-1.623531477016908
N	5.194022938670292	1.423812513514112	1.190861442521122
N	-1.516240596985753	-4.970186648213890	-1.710260442219688
N	1.473862549957790	-5.191547431783544	-0.990090956633196
N	-3.113696914256476	3.565235787015252	0.789406253932080
N	3.579092000510210	3.219561370175268	-0.353339121802051
N	-3.526111549374015	-3.128197035639289	-0.764442908841684
N	3.193722961405834	-3.581516329038873	0.665321788450296
H	-1.282359774312816	-5.912795569889489	-1.384269378002248
H	-1.403772751021897	-4.959899695745060	-2.729909896154382
H	-3.191561537733179	-3.996838737440513	-1.198074420128084
H	-4.308300946575461	-2.704268861440035	-1.262727275023018
H	-5.013600324525394	1.770497780553928	2.433769069476310
H	-5.995316606154033	1.159581898948358	1.244116078718670
H	-0.996930084043850	6.117939015693126	-0.687735560581679
H	2.001627423128414	4.592598734299612	-2.494697388247996
H	1.058279810683960	5.788877405134400	-1.863563022495864
H	3.290076480783446	4.137233689670774	-0.693595109230081
H	4.440599773102966	2.879440933463382	-0.777305069111755
H	4.929635271880700	2.402158438962380	1.321488362903522
H	5.713377607455122	1.082332484843322	2.001888902124166
H	5.946883400663482	-1.319689418513313	1.475322436203538
H	4.935811505791016	-1.592579411758472	2.759164729311874
H	4.067917863378754	-3.260410860492264	1.098365753023882
H	2.789416192573916	-4.385833323374193	1.145279830457498
H	2.468379721424920	-4.955636165920559	-0.974694118542594
H	1.223848537302450	-5.681642965560371	-1.850639606327512
H	-4.992177216985992	-2.411796278498418	0.795017650177174
H	-5.749345701536981	-1.184574613179205	1.644426256558054
H	-4.104439154711477	3.319137294540108	0.846320718347820
H	-2.869455091573311	4.472677280464650	0.385921195706086
H	-1.760208645196006	5.268333817580694	-1.887532362475920
H	-1.279170597743612	0.629357938346084	3.260926458126172
O	0.250595054682634	-0.012492256731048	2.332678743230254
O	-0.918511087762891	-0.274572428368739	3.128163804501882

Transition Metal: Ni; Functional Group: OH; Adsorbate: Clean

Ni	11.000420000000000	11.014150000000001	7.875650000000000
C	10.353289999999999	15.167479999999999	7.514540000000000
C	9.946149999999999	13.792550000000000	7.492700000000000
C	8.633450000000000	13.357570000000001	7.289000000000000
C	11.630170000000000	6.861800000000000	7.501310000000000
C	12.051780000000001	8.233620000000000	7.512290000000000
C	13.377140000000001	8.657000000000000	7.379940000000000
C	10.328270000000000	6.817570000000000	7.945840000000000
C	9.921490000000000	8.191750000000001	8.136110000000000
C	11.667880000000000	15.212199999999999	7.920090000000000
C	8.613530000000001	8.618370000000001	8.412400000000000
C	15.154430000000000	11.644230000000000	8.271430000000001
C	12.073969999999999	13.839919999999999	8.121090000000001
C	13.783770000000001	12.085110000000000	8.253270000000001
C	15.175620000000000	10.333510000000000	7.865100000000000
C	13.798159999999999	9.956200000000001	7.656800000000000
C	13.378399999999999	13.416150000000000	8.419710000000000
C	6.824730000000000	11.678739999999999	7.729160000000000
C	8.207030000000000	12.059880000000000	7.567120000000000
C	6.837590000000000	10.380580000000000	8.175810000000000
C	8.210080000000000	9.946940000000000	8.217650000000001
N	11.008620000000001	12.977660000000000	7.858360000000000
N	10.990010000000000	9.051250000000000	7.874390000000000
N	12.948930000000001	11.030469999999999	7.890580000000000
N	9.052170000000000	10.997150000000000	7.860900000000000
O	9.532170000000001	16.261060000000001	7.176060000000000
O	7.647060000000000	14.258770000000000	6.901980000000000
O	12.453090000000000	5.747240000000000	7.231970000000000
O	14.379730000000000	7.738060000000000	7.076360000000000
O	9.546189999999999	5.710280000000000	8.135050000000000
O	12.456640000000000	16.322179999999999	8.086710000000000
O	7.711750000000000	7.654350000000000	8.782660000000000
O	16.222030000000000	12.461620000000000	8.609170000000001
O	16.310770000000002	9.573119999999999	7.737590000000000
O	14.272620000000000	14.384800000000000	8.797090000000001
O	5.691000000000000	12.429560000000000	7.541590000000000
O	5.763270000000000	9.566879999999999	8.501700000000000
H	9.379420000000000	16.798760000000001	7.977780000000000
H	8.053280000000001	15.154590000000001	6.853730000000000
H	12.292949999999999	5.455810000000000	6.313140000000000
H	13.992279999999999	6.834750000000000	7.137720000000000
H	10.122240000000000	4.929150000000000	8.020910000000001
H	12.016019999999999	17.065550000000002	7.631100000000000
H	6.814240000000000	8.048470000000000	8.803780000000000
H	17.052389999999999	11.981140000000000	8.434350000000000
H	16.021339999999999	8.676090000000000	7.464320000000000
H	15.169370000000001	13.990930000000001	8.842250000000000
H	5.981760000000000	13.313520000000000	7.231650000000000
H	4.937300000000000	10.026430000000000	8.261939999999999

Transition Metal: Ni; Functional Group: OH; Adsorbate: O

Ni	10.994510000000000	11.013170000000001	7.675210000000000
C	10.326359999999999	15.250209999999999	6.967050000000000
C	9.919029999999999	13.872900000000000	6.991930000000000
C	8.588360000000000	13.423150000000000	6.896270000000000
C	11.661239999999999	6.780240000000000	6.928830000000000
C	12.075670000000001	8.154190000000000	7.000760000000000
C	13.411619999999999	8.596410000000001	6.970010000000000
C	10.298710000000000	6.736450000000000	7.139860000000000
C	9.872460000000000	8.113560000000000	7.281170000000000
C	11.695750000000000	15.290210000000000	7.130140000000000
C	8.538489999999999	8.557930000000001	7.428420000000000
C	15.239020000000000	11.680490000000001	7.374070000000000
C	12.122180000000000	13.912929999999999	7.266280000000000
C	13.867270000000000	12.121340000000000	7.356570000000000
C	15.241360000000000	10.315700000000000	7.197030000000000
C	13.854290000000001	9.921690000000000	7.101980000000000
C	13.454920000000000	13.469910000000000	7.426690000000000
C	6.755960000000000	11.701440000000000	7.078680000000000
C	8.144880000000001	12.098360000000000	7.029400000000000
C	6.754540000000000	10.342770000000000	7.295900000000000
C	8.127020000000000	9.905650000000000	7.335700000000000
N	11.027550000000000	13.067280000000000	7.163280000000000
N	10.968550000000000	8.958920000000001	7.185650000000000
N	13.028210000000000	11.030080000000000	7.186020000000000
N	8.969220000000000	10.994680000000001	7.170980000000000
O	10.977969999999999	11.013719999999999	9.411410000000000
O	9.477900000000000	16.354859999999999	6.745170000000000
O	7.580150000000000	14.357110000000000	6.693960000000000
O	12.508240000000001	5.665140000000000	6.751660000000000
O	14.424630000000001	7.653170000000000	6.843530000000000
O	9.499680000000000	5.626060000000000	7.172450000000000
O	12.499050000000000	16.399719999999999	7.137900000000000
O	7.606210000000000	7.573600000000000	7.614650000000000
O	16.327200000000001	12.525639999999999	7.512160000000000
O	16.379439999999999	9.553210000000000	7.127900000000000
O	14.383360000000000	14.456070000000000	7.622430000000000
O	5.619220000000000	12.457750000000001	6.946880000000000
O	5.664130000000000	9.498550000000000	7.422820000000000
H	9.420210000000001	16.877220000000001	7.569120000000000
H	7.992180000000000	15.248810000000001	6.611650000000000
H	12.430120000000001	5.356150000000000	5.827590000000000
H	14.018000000000001	6.755320000000000	6.848860000000000
H	10.087640000000000	4.845320000000000	7.162990000000000
H	11.972980000000000	17.145849999999999	6.789320000000000
H	6.709310000000000	7.971200000000000	7.618940000000000
H	17.145980000000002	12.000980000000000	7.437750000000000
H	16.092500000000001	8.622430000000000	7.016290000000000
H	15.279540000000001	14.058320000000000	7.652580000000000
H	5.907620000000000	13.382860000000001	6.798630000000000
H	4.847770000000000	10.011590000000000	7.275390000000000

Transition Metal: Ni; Functional Group: OH; Adsorbate: OH

Ni	10.995799999999999	11.013820000000001	7.307680000000000
C	10.316260000000000	15.262449999999999	6.730150000000000
C	9.912390000000000	13.886130000000000	6.830650000000000
C	8.582760000000000	13.423170000000001	6.829340000000000
C	11.674810000000001	6.759600000000000	6.687620000000000
C	12.082570000000000	8.128100000000000	6.850780000000000
C	13.413740000000001	8.585070000000000	6.906860000000000
C	10.303640000000000	6.711770000000000	6.839830000000000
C	9.881600000000001	8.082420000000001	7.048370000000000
C	11.690379999999999	15.301990000000000	6.844710000000000
C	8.554040000000001	8.537610000000001	7.228040000000000
C	15.187560000000000	11.673069999999999	7.460890000000000
C	12.108940000000000	13.926850000000000	7.038760000000000
C	13.826919999999999	12.116809999999999	7.288500000000000
C	15.204020000000000	10.307150000000000	7.314850000000000
C	13.833030000000001	9.912620000000000	7.082990000000000
C	13.430650000000000	13.473290000000000	7.260530000000000
C	6.779780000000000	11.700979999999999	7.174800000000000
C	8.160050000000000	12.094820000000000	7.001770000000000
C	6.791000000000000	10.337690000000000	7.343350000000000
C	8.158180000000000	9.894310000000001	7.236400000000000
N	11.015630000000000	13.084360000000000	7.008600000000000
N	10.978000000000000	8.926940000000000	7.049660000000000
N	12.999459999999999	11.026020000000001	7.051970000000000
N	8.994640000000000	10.984740000000000	7.023900000000000
O	10.992640000000000	11.081460000000000	9.226630000000000
O	9.450620000000001	16.355100000000000	6.512680000000000
O	7.561510000000000	14.347799999999999	6.684470000000000
O	12.531650000000001	5.652160000000000	6.505880000000000
O	14.435969999999999	7.650800000000000	6.826230000000000
O	9.496309999999999	5.607440000000000	6.788440000000000
O	12.505710000000001	16.403120000000001	6.786300000000000
O	7.614290000000000	7.557900000000000	7.366890000000000
O	16.260210000000001	12.518760000000000	7.696160000000000
O	16.342630000000000	9.543780000000000	7.387310000000000
O	14.362640000000001	14.453659999999999	7.435930000000000
O	5.638500000000000	12.462619999999999	7.181030000000000
O	5.709950000000000	9.493010000000000	7.545590000000000
H	11.036500000000000	10.155239999999999	9.532780000000001
H	9.466030000000000	16.927949999999999	7.304520000000000
H	7.963540000000000	15.241450000000000	6.567520000000000
H	12.523190000000000	5.398310000000000	5.562100000000000
H	14.034120000000000	6.751220000000000	6.784060000000000
H	10.077790000000000	4.822320000000000	6.759380000000000
H	11.980729999999999	17.140370000000001	6.418030000000000
H	6.723260000000000	7.965680000000000	7.438210000000000
H	17.084620000000001	11.997800000000000	7.675930000000000
H	16.076280000000001	8.614590000000000	7.227270000000000
H	15.250310000000001	14.047820000000000	7.546600000000000
H	5.909720000000000	13.387480000000000	7.004850000000000
H	4.885920000000000	10.007920000000000	7.459360000000000

Transition Metal: Ni; Functional Group: OH; Adsorbate: OOH

Ni	10.982519999999999	11.037910000000000	6.687350000000000
C	10.320280000000000	15.310370000000001	6.199690000000000
C	9.913750000000000	13.931699999999999	6.246860000000000
C	8.580660000000000	13.476010000000000	6.215210000000000
C	11.649649999999999	6.777910000000000	6.188510000000000
C	12.059220000000000	8.154120000000001	6.271680000000000
C	13.394090000000000	8.603970000000000	6.305360000000000
C	10.278190000000000	6.741270000000000	6.328380000000000
C	9.857440000000000	8.124129999999999	6.448660000000000
C	11.695810000000000	15.343299999999999	6.293770000000000
C	8.527100000000001	8.585910000000000	6.588940000000000
C	15.210419999999999	11.695660000000000	6.675800000000000
C	12.115340000000000	13.960360000000000	6.419980000000000
C	13.842440000000000	12.140300000000000	6.570550000000000
C	15.213329999999999	10.326000000000001	6.571300000000000
C	13.829760000000000	9.933880000000000	6.419120000000000
C	13.444940000000001	13.497900000000000	6.572000000000000
C	6.755150000000000	11.754600000000000	6.452450000000000
C	8.142799999999999	12.147349999999999	6.346030000000000
C	6.756000000000000	10.388870000000001	6.609760000000000
C	8.126899999999999	9.943709999999999	6.566110000000000
H	9.452230000000000	16.935659999999999	6.861330000000000
H	7.976360000000000	15.305149999999999	5.987780000000000
H	12.477160000000000	5.333040000000000	5.156340000000000
H	14.000560000000000	6.761400000000000	6.260280000000000
H	10.054040000000001	4.851800000000000	6.397990000000000
H	11.971590000000001	17.202590000000001	5.963270000000000
H	6.687920000000000	8.020360000000000	6.747840000000000
H	17.115790000000001	12.009270000000001	6.821110000000000
H	16.069230000000001	8.625190000000000	6.514440000000000
H	15.278470000000000	14.066860000000000	6.778590000000000
H	5.897670000000000	13.445440000000000	6.262880000000000
H	4.846570000000000	10.062840000000000	6.631320000000000
H	9.466790000000000	10.577550000000000	9.455850000000000
O	9.459270000000000	16.416509999999999	6.033260000000000
O	7.566380000000000	14.411540000000000	6.073410000000000
O	12.505530000000000	5.660350000000000	6.076770000000000
O	14.408440000000001	7.659600000000000	6.259770000000000
O	9.471710000000000	5.634560000000000	6.339280000000000
O	12.509340000000000	16.446100000000001	6.268780000000000
O	7.579920000000000	7.610330000000000	6.712870000000000
O	16.298649999999999	12.541729999999999	6.826240000000000
O	16.350899999999999	9.558870000000001	6.608920000000000
O	14.387779999999999	14.475330000000000	6.710390000000000
O	5.615700000000000	12.519520000000000	6.416400000000000
O	5.664020000000000	9.545460000000000	6.756220000000000
O	11.044800000000000	11.218460000000000	8.612570000000000
O	10.359180000000000	10.183890000000000	9.332920000000000
N	11.018710000000000	13.120820000000000	6.374780000000000
N	10.954620000000000	8.964230000000001	6.406150000000000
N	13.001340000000001	11.048069999999999	6.404030000000000
N	8.971780000000001	11.033569999999999	6.403350000000000

Systems with explicit solvation

Transition Metal: Co; Functional Group: F; Adsorbate: OH

C	9.111700000000001	15.228149999999999	8.170290000000000
C	9.001260000000000	13.855390000000000	8.593880000000000
C	8.919720000000000	13.429670000000000	9.914690000000000
C	8.974750000000000	6.769770000000000	6.827010000000000
C	8.917130000000000	8.147420000000000	6.405760000000000
C	8.840249999999999	8.573740000000001	5.085590000000000
C	9.001170000000000	6.774110000000000	8.193149999999999
C	8.959600000000000	8.154299999999999	8.607870000000000
C	9.114640000000000	15.224700000000000	6.803140000000000
C	8.916040000000001	8.589110000000000	9.927060000000001
C	8.697329999999999	11.675870000000000	3.274640000000000
C	9.007770000000001	13.849589999999999	6.387270000000000
C	8.814930000000000	12.097650000000000	4.648210000000000
C	8.676010000000000	10.310010000000000	3.279880000000000
C	8.777180000000000	9.894230000000000	4.657170000000000
C	8.930440000000001	13.416700000000001	5.068710000000000
C	8.705060000000000	11.696709999999999	11.720430000000000
C	8.811180000000000	12.112909999999999	10.343740000000000
C	8.711119999999999	10.330850000000000	11.723390000000000
C	8.818830000000000	9.909640000000000	10.348610000000001
Co	9.062820000000000	11.004830000000000	7.498900000000000
F	8.599550000000001	12.472950000000001	2.197260000000000
F	8.559229999999999	9.510680000000001	2.207130000000000
F	9.177780000000000	16.299820000000000	5.999380000000000
F	9.176230000000000	16.308479999999999	8.967820000000000
F	8.594300000000000	12.497130000000000	12.793650000000000
F	8.970430000000000	5.689110000000000	6.030120000000000
F	9.018950000000000	5.698560000000000	8.998460000000000
F	8.963570000000001	14.371729999999999	4.102830000000000
F	8.951870000000000	14.390779999999999	10.874910000000000
F	8.814069999999999	7.613950000000000	4.127090000000000
F	8.955500000000001	7.635790000000000	10.893720000000000
F	8.602700000000000	9.533239999999999	12.798719999999999
H	11.232889999999999	11.916670000000000	7.413300000000000
H	13.049740000000000	14.146739999999999	8.467520000000000
H	12.050310000000000	10.726210000000000	8.995320000000000
H	13.424870000000000	10.235099999999999	9.539999999999999
H	13.047710000000000	12.612230000000000	8.745990000000001
H	11.980540000000000	9.843640000000001	6.419520000000000
H	13.240500000000001	9.590970000000000	5.546960000000000
O	10.935969999999999	10.984900000000000	7.506530000000000
O	12.756309999999999	10.931880000000000	9.660580000000000
O	12.504740000000000	9.129479999999999	5.984420000000000
O	12.851680000000000	13.289260000000001	8.054819999999999
N	8.934170000000000	13.004049999999999	7.492760000000000
N	8.899319999999999	9.000579999999999	7.504620000000000
N	8.824590000000001	10.998220000000000	5.503610000000000
N	8.833830000000001	11.008860000000000	9.494940000000000

Transition Metal: Co; Functional Group: F; Adsorbate: OOH

C	8.587320000000000	15.218970000000001	8.212199999999999
C	8.592950000000000	13.836710000000000	8.623740000000000
C	8.558800000000000	13.396750000000001	9.942040000000000
C	8.735740000000000	6.755070000000000	6.810860000000000
C	8.711040000000001	8.137810000000000	6.399390000000000
C	8.746589999999999	8.576510000000001	5.080690000000000
C	8.713469999999999	6.748340000000000	8.177080000000000
C	8.666150000000000	8.126939999999999	8.601440000000000
C	8.618679999999999	15.226000000000001	6.845400000000000
C	8.626070000000000	8.552190000000000	9.924390000000001
C	8.764210000000000	11.689240000000000	3.282010000000000
C	8.654840000000000	13.848520000000001	6.419790000000000
C	8.738490000000001	12.103990000000000	4.663330000000000
C	8.764490000000000	10.323460000000001	3.277600000000000
C	8.743280000000000	9.899990000000001	4.656640000000000
C	8.719580000000001	13.423190000000000	5.098300000000000
C	8.481750000000000	11.650589999999999	11.744420000000000
C	8.525880000000001	12.074070000000001	10.366230000000000
C	8.519890000000000	10.285140000000000	11.740449999999999
C	8.571520000000000	9.871470000000000	10.358610000000001
Co	8.824290000000000	10.993790000000001	7.524950000000000
F	8.764410000000000	12.491220000000000	2.203270000000000
F	8.766140000000000	9.529050000000000	2.193800000000000
F	8.597920000000000	16.310739999999999	6.048980000000000
F	8.537530000000000	16.295339999999999	9.016670000000000
F	8.399380000000001	12.446080000000000	12.825170000000000
F	8.765919999999999	5.679680000000000	6.003870000000000
F	8.722110000000001	5.664270000000000	8.971410000000001
F	8.762180000000001	14.391090000000000	4.141500000000000
F	8.548579999999999	14.353970000000000	10.907819999999999
F	8.786490000000001	7.620630000000000	4.114000000000000
F	8.628110000000000	7.588510000000000	10.881900000000000
F	8.500540000000001	9.483950000000000	12.818809999999999
H	12.844749999999999	12.698399999999999	6.158780000000000
H	12.542940000000000	10.198440000000000	9.451680000000000
H	13.573810000000000	9.652120000000000	10.461449999999999
H	12.382059999999999	14.187480000000001	6.353830000000000
H	11.952450000000001	10.743530000000000	6.057360000000000
H	13.373849999999999	10.377390000000000	5.544940000000000
H	11.723000000000001	12.453960000000000	7.942410000000000
O	10.699769999999999	10.860849999999999	7.583040000000000
O	13.024050000000001	9.385570000000000	9.704660000000001
O	12.642560000000000	11.004730000000000	5.404430000000000
O	12.694110000000000	13.404610000000000	6.838510000000000
O	11.334899999999999	11.728960000000001	8.526230000000000
N	8.619990000000000	12.993670000000000	7.518000000000000
N	8.649030000000000	8.980200000000000	7.504100000000000
N	8.712160000000001	10.999350000000000	5.510860000000000
N	8.554610000000000	10.976310000000000	9.514260000000000

Transition Metal: Co; Functional Group: H; Adsorbate: OH

Co	5.681080000000000	11.014160000000000	10.985160000000000
H	5.121070000000000	12.360889999999999	5.924860000000000
H	5.080690000000000	9.631280000000000	5.940660000000000
H	5.619670000000000	16.081669999999999	9.600330000000000
H	5.632170000000000	16.091560000000001	12.329590000000000
H	5.229280000000000	12.402040000000000	16.045430000000000
H	5.510220000000000	5.939700000000000	9.641610000000000
H	5.560800000000000	5.948270000000000	12.370860000000000
H	5.426720000000000	14.202950000000000	7.773420000000000
H	5.467500000000000	14.229200000000001	14.171860000000001
H	5.335350000000000	7.803890000000000	7.806320000000000
H	5.441030000000000	7.828390000000000	14.199500000000000
H	5.223750000000000	9.673109999999999	16.057130000000001
H	7.953460000000000	11.890120000000000	10.842359999999999
H	9.456329999999999	14.173909999999999	12.057510000000001
H	8.689090000000000	10.769180000000000	12.491360000000000
H	10.050390000000000	10.310900000000000	13.086670000000000
H	9.726910000000000	12.658230000000000	12.259270000000001
H	8.628740000000001	9.759919999999999	9.910620000000000
H	9.885880000000000	9.643540000000000	9.015350000000000
C	5.619940000000000	15.239780000000000	11.652100000000001
C	5.571580000000000	13.857559999999999	12.076919999999999
C	5.467730000000000	13.454359999999999	13.403910000000000
C	5.522860000000000	6.789510000000000	10.320830000000001
C	5.489690000000000	8.173890000000000	9.898099999999999
C	5.360660000000000	8.577790000000000	8.574930000000000
C	5.549600000000000	6.794090000000000	11.686590000000001
C	5.531340000000000	8.181580000000000	12.100500000000000
C	5.613260000000000	15.235130000000000	10.284480000000000
C	5.444840000000000	8.596159999999999	13.424429999999999
C	5.169210000000000	11.685680000000000	6.776570000000000
C	5.557930000000000	13.849930000000001	9.870550000000000
C	5.292720000000000	12.109410000000000	8.150230000000001
C	5.147180000000000	10.315580000000001	6.784460000000000
C	5.258870000000000	9.903330000000000	8.163190000000000
C	5.431290000000000	13.435499999999999	8.548959999999999
C	5.263700000000000	11.719379999999999	15.198930000000001
C	5.350350000000000	12.131250000000000	13.818669999999999
C	5.260620000000000	10.349060000000000	15.204879999999999
C	5.343110000000000	9.924620000000001	13.827890000000000
O	7.610660000000000	10.978740000000000	10.967660000000000
O	9.357320000000000	10.985390000000001	13.193220000000000
O	9.171840000000000	9.109040000000000	9.402380000000001
O	9.673170000000001	13.361810000000000	11.568890000000000
N	5.562530000000000	13.012680000000000	10.976810000000000
N	5.522950000000000	9.018129999999999	10.996060000000000
N	5.311810000000000	11.010370000000000	8.997859999999999
N	5.362110000000000	11.024470000000001	12.981760000000000

Transition Metal: Co; Functional Group: H; Adsorbate: OOH

Co	5.433880000000000	11.008559999999999	11.021550000000000
H	5.368670000000000	12.410800000000000	5.949610000000000
H	5.346650000000000	9.680740000000000	5.932220000000000
H	5.243180000000000	16.091670000000001	9.681410000000000
H	5.129300000000000	16.067820000000001	12.409110000000000
H	5.039830000000000	12.334510000000000	16.085560000000001
H	5.298110000000000	5.946330000000000	9.607900000000001
H	5.263020000000000	5.927080000000000	12.339689999999999
H	5.371910000000000	14.232340000000001	7.833140000000000
H	5.117610000000000	14.180840000000000	14.229460000000000
H	5.347720000000000	7.834120000000000	7.789420000000000
H	5.246730000000000	7.785930000000000	14.186500000000001
H	5.103450000000000	9.603730000000001	16.066690000000001
H	9.451230000000001	12.676399999999999	9.723409999999999
H	9.115900000000000	10.107920000000000	12.927930000000000
H	10.164389999999999	9.787229999999999	14.009119999999999
H	8.777300000000000	14.073890000000000	9.897150000000000
H	8.476630000000000	10.785030000000001	9.562910000000000
H	9.916119999999999	10.336360000000001	9.198820000000000
H	8.356960000000001	12.385400000000001	11.492110000000000
C	5.192850000000000	15.225320000000000	11.723030000000000
C	5.210450000000000	13.838500000000000	12.129350000000001
C	5.157350000000000	13.415360000000000	13.452360000000001
C	5.288650000000000	6.788730000000000	10.296650000000000
C	5.290110000000000	8.177519999999999	9.890720000000000
C	5.328320000000000	8.599570000000000	8.567019999999999
C	5.270020000000000	6.779100000000000	11.663340000000000
C	5.255110000000000	8.160729999999999	12.089820000000000
C	5.252850000000000	15.237209999999999	10.355960000000000
C	5.234080000000000	8.561950000000000	13.419710000000000
C	5.364290000000000	11.723260000000000	6.793490000000000
C	5.305490000000000	13.856660000000000	9.929720000000000
C	5.359610000000000	12.130490000000000	8.180210000000001
C	5.352020000000000	10.356460000000000	6.784960000000000
C	5.341050000000000	9.930149999999999	8.165880000000000
C	5.356000000000000	13.455150000000000	8.599760000000000
C	5.092340000000000	11.659060000000000	15.233890000000001
C	5.142630000000000	12.085150000000001	13.852790000000001
C	5.123220000000000	10.292430000000000	15.224390000000000
C	5.185940000000000	9.885949999999999	13.837930000000000
O	7.300820000000000	10.832660000000001	11.055470000000000
O	9.674550000000000	9.380820000000000	13.273650000000000
O	9.232609999999999	10.986179999999999	8.957060000000000
O	9.311030000000001	13.413910000000000	10.372930000000000
O	7.972620000000000	11.634630000000000	12.039540000000001
N	5.272920000000000	13.000450000000001	11.023750000000000
N	5.251140000000000	9.014609999999999	10.996600000000001
N	5.334180000000000	11.024620000000001	9.021260000000000
N	5.180560000000000	10.991289999999999	12.999820000000000

Transition Metal: Cr; Functional Group: F; Adsorbate: OH

C	8.923730000000001	15.249120000000000	8.162820000000000
C	8.918130000000000	13.873910000000000	8.589980000000001
C	8.923389999999999	13.422750000000001	9.913950000000000
C	8.798990000000000	6.725190000000000	6.791130000000000
C	8.850009999999999	8.100030000000000	6.364320000000000
C	8.880890000000001	8.550459999999999	5.039500000000000
C	8.801869999999999	6.724700000000000	8.164389999999999
C	8.855490000000000	8.100059999999999	8.589969999999999
C	8.928490000000000	15.248120000000000	6.789990000000000
C	8.894439999999999	8.551570000000000	9.913779999999999
C	8.924799999999999	11.670120000000001	3.209490000000000
C	8.925459999999999	13.871840000000001	6.364420000000000
C	8.914170000000000	12.096159999999999	4.586830000000000
C	8.914239999999999	10.298489999999999	3.208940000000000
C	8.891990000000000	9.873329999999999	4.587130000000000
C	8.934290000000001	13.418630000000000	5.040470000000000
C	8.928290000000001	11.674580000000001	11.745939999999999
C	8.910470000000000	12.100090000000000	10.368209999999999
C	8.927600000000000	10.301890000000000	11.745970000000000
C	8.905810000000001	9.874820000000000	10.368340000000000
F	8.935530000000000	9.512250000000000	12.834180000000000
F	8.936109999999999	12.461440000000000	2.123380000000000
F	8.915660000000001	9.510350000000001	2.121420000000000
F	8.929790000000001	16.334610000000001	5.998480000000000
F	8.919890000000001	16.336150000000000	8.952260000000001
F	8.940849999999999	12.463369999999999	12.834120000000000
F	8.743110000000000	5.640150000000000	6.000340000000000
F	8.749770000000000	5.638480000000000	8.955180000000000
F	8.963699999999999	14.384499999999999	4.080250000000000
F	8.943920000000000	14.386160000000000	10.876849999999999
F	8.897810000000000	7.587810000000000	4.079110000000000
F	8.919710000000000	7.585420000000000	10.875410000000000
H	11.427519999999999	11.881360000000001	7.491650000000000
H	13.365629999999999	13.507910000000001	7.421300000000000
H	12.413330000000000	10.514880000000000	8.834180000000000
H	13.140739999999999	10.448380000000000	10.215619999999999
H	13.106830000000000	12.573070000000000	8.635910000000001
H	11.967960000000000	10.136870000000000	5.994510000000000
H	13.222400000000000	9.399190000000001	5.461860000000000
O	11.044630000000000	10.967770000000000	7.481740000000000
O	13.256550000000001	10.737909999999999	9.294940000000000
O	12.366740000000000	9.761469999999999	5.175270000000000
O	12.679610000000000	13.252630000000000	8.062350000000000
N	8.912310000000000	13.037509999999999	7.477880000000000
N	8.872529999999999	8.934799999999999	7.476910000000000
N	8.884700000000000	10.984610000000000	5.421900000000000
N	8.888980000000000	10.987520000000000	9.534340000000000
Cr	9.172340000000000	10.985530000000001	7.476420000000000

Transition Metal: Cr; Functional Group: F; Adsorbate: OOH

C	8.827690000000000	15.248519999999999	8.217790000000001
C	8.780680000000000	13.870039999999999	8.636139999999999
C	8.727069999999999	13.409770000000000	9.956510000000000
C	8.446600000000000	6.733910000000000	6.796450000000000
C	8.544240000000000	8.110670000000001	6.379000000000000
C	8.586390000000000	8.569670000000000	5.057920000000000
C	8.454630000000000	6.725120000000000	8.169160000000000
C	8.551850000000000	8.096900000000000	8.602700000000000
C	8.893070000000000	15.255120000000000	6.846090000000000
C	8.582860000000000	8.539990000000000	9.929840000000000
C	8.766930000000000	11.697340000000001	3.246520000000000
C	8.874070000000000	13.880739999999999	6.411750000000000
C	8.817740000000001	12.114120000000000	4.625820000000000
C	8.670660000000000	10.328329999999999	3.239000000000000
C	8.666850000000000	9.893829999999999	4.613710000000000
C	8.895860000000001	13.432779999999999	5.086200000000000
C	8.614879999999999	11.653430000000000	11.776090000000000
C	8.662520000000001	12.085390000000000	10.401759999999999
C	8.593550000000000	10.280980000000000	11.769780000000001
C	8.614120000000000	9.860920000000000	10.390689999999999
F	8.544190000000000	9.489739999999999	12.854340000000001
F	8.780030000000000	12.492960000000000	2.163200000000000
F	8.574439999999999	9.549540000000000	2.147980000000000
F	8.943090000000000	16.346430000000002	6.060560000000000
F	8.794930000000001	16.331930000000000	9.013610000000000
F	8.585649999999999	12.438770000000000	12.866690000000000
F	8.350590000000000	5.656890000000000	5.997380000000000
F	8.362480000000000	5.637930000000000	8.953650000000000
F	8.975330000000000	14.400320000000001	4.128390000000000
F	8.735160000000000	14.368729999999999	10.924490000000000
F	8.535050000000000	7.614020000000000	4.088070000000000
F	8.556580000000000	7.572210000000000	10.885820000000001
H	13.358120000000000	12.261960000000000	6.308170000000000
H	12.455750000000000	9.971900000000000	9.476419999999999
H	13.334390000000001	9.275029999999999	10.540960000000000
H	13.054300000000000	13.796900000000001	6.419440000000000
H	12.256019999999999	10.407560000000000	6.156910000000000
H	13.662250000000000	9.880960000000000	5.758000000000000
H	12.073060000000000	12.212020000000001	7.996880000000000
O	10.866860000000001	10.786500000000000	7.500880000000000
O	12.769600000000001	9.091540000000000	9.771129999999999
O	13.020410000000000	10.586140000000000	5.562430000000000
O	13.258599999999999	13.009570000000000	6.952120000000000
O	11.525060000000000	11.572630000000000	8.546680000000000
N	8.802210000000001	13.042410000000000	7.519540000000000
N	8.596180000000000	8.936550000000000	7.495740000000000
N	8.750710000000000	10.998460000000000	5.455110000000000
N	8.651080000000000	10.977390000000000	9.563219999999999
Cr	8.996409999999999	10.979699999999999	7.521210000000000

Transition Metal: Cr; Functional Group: H; Adsorbate: OH

Cr	5.498780000000000	10.988550000000000	10.987100000000000
C	5.280460000000000	15.247900000000000	11.678850000000001
C	5.282570000000000	13.864910000000000	12.101570000000001
C	5.269770000000000	13.429240000000000	13.431580000000000
C	5.081690000000000	6.740860000000000	10.301950000000000
C	5.142360000000000	8.122660000000000	9.879330000000000
C	5.128120000000000	8.557800000000000	8.550620000000000
C	5.093960000000000	6.739100000000000	11.673610000000000
C	5.162690000000000	8.120649999999999	12.098330000000001
C	5.271360000000000	15.249730000000000	10.306509999999999
C	5.171180000000000	8.553410000000000	13.428559999999999
C	5.126660000000000	11.682210000000000	6.733730000000000
C	5.266870000000000	13.867940000000001	9.880720000000000
C	5.190270000000000	12.105300000000000	8.117030000000000
C	5.096390000000000	10.311439999999999	6.735030000000000
C	5.141850000000000	9.887440000000000	8.117920000000000
C	5.235410000000000	13.434030000000000	8.550500000000000
C	5.186070000000000	11.676539999999999	15.247719999999999
C	5.234500000000000	12.100110000000001	13.864340000000000
C	5.159070000000000	10.305920000000000	15.246610000000000
C	5.190940000000000	9.882569999999999	13.863160000000001
N	5.274470000000000	13.032340000000000	10.990110000000000
N	5.192650000000000	8.954520000000000	10.989380000000001
N	5.192060000000000	10.995810000000001	8.950609999999999
N	5.230300000000000	10.991160000000001	13.030130000000000
O	7.383720000000000	10.973290000000000	10.968340000000000
O	9.340140000000000	10.982600000000000	13.008730000000000
O	8.963530000000000	9.302049999999999	9.170059999999999
O	9.347510000000000	13.222540000000000	11.203260000000000
H	5.116670000000000	9.632389999999999	16.100200000000001
H	5.104900000000000	12.355200000000000	5.878620000000000
H	5.046120000000000	9.637650000000001	5.881740000000000
H	5.259840000000000	16.105789999999999	9.634539999999999
H	5.275120000000000	16.102570000000000	12.352800000000000
H	5.171710000000000	12.349620000000000	16.102950000000000
H	5.030860000000000	5.888320000000000	9.627219999999999
H	5.053090000000000	5.884540000000000	12.346290000000000
H	5.231510000000000	14.206980000000000	7.778920000000000
H	5.271640000000000	14.201210000000000	14.204280000000001
H	5.096200000000000	7.786480000000000	7.778560000000000
H	5.143610000000000	7.780590000000000	14.199640000000000
H	7.748070000000000	11.874800000000000	10.815670000000001
H	9.129370000000000	14.054259999999999	11.657719999999999
H	8.575120000000000	10.759150000000000	12.417669999999999
H	9.998600000000000	10.290020000000000	12.825329999999999
H	9.557140000000000	12.585770000000000	11.929510000000001
H	8.392650000000000	9.874650000000001	9.735670000000001
H	9.518520000000001	9.931480000000001	8.678970000000000

Transition Metal: Cr; Functional Group: H; Adsorbate: OOH

Cr	5.720630000000000	10.978280000000000	11.021910000000000
C	5.550280000000000	15.240200000000000	11.740910000000000
C	5.528720000000000	13.853030000000000	12.151660000000000
C	5.480050000000000	13.405490000000000	13.476760000000001
C	5.198980000000000	6.743170000000000	10.288919999999999
C	5.293530000000000	8.129140000000000	9.879239999999999
C	5.316790000000000	8.575810000000001	8.553730000000000
C	5.188860000000000	6.730710000000000	11.659789999999999
C	5.275610000000000	8.108670000000000	12.095980000000001
C	5.566270000000000	15.253080000000001	10.368220000000001
C	5.273060000000000	8.530810000000001	13.429240000000000
C	5.412870000000000	11.716989999999999	6.765740000000000
C	5.554610000000000	13.872940000000000	9.931660000000001
C	5.477970000000000	12.125190000000000	8.152320000000000
C	5.348220000000000	10.346950000000000	6.753440000000000
C	5.373540000000000	9.909190000000001	8.132500000000000
C	5.539850000000000	13.450070000000000	8.597239999999999
C	5.317010000000000	11.639780000000000	15.274260000000000
C	5.404840000000000	12.073140000000000	13.896190000000001
C	5.261280000000000	10.269130000000001	15.261500000000000
C	5.312800000000000	9.856560000000000	13.874980000000001
N	5.536080000000000	13.030090000000000	11.034470000000001
N	5.337510000000000	8.949859999999999	10.995460000000000
N	5.450440000000000	11.008089999999999	8.976200000000000
N	5.396020000000000	10.971120000000001	13.054029999999999
O	7.600600000000000	10.785980000000000	10.920710000000000
O	9.704800000000001	9.415340000000000	13.770200000000001
O	9.386049999999999	11.239860000000000	8.731590000000001
O	9.475730000000000	13.491630000000001	10.447699999999999
O	8.306410000000000	11.464399999999999	12.010149999999999
H	5.179960000000000	9.591650000000000	16.109310000000001
H	5.412010000000000	12.399509999999999	5.918140000000000
H	5.286410000000000	9.682950000000000	5.893270000000000
H	5.566830000000000	16.114999999999998	9.703160000000000
H	5.538040000000000	16.089140000000000	12.422079999999999
H	5.293420000000000	12.305569999999999	16.134950000000000
H	5.141960000000000	5.896430000000000	9.607580000000000
H	5.122830000000000	5.872120000000000	12.325260000000000
H	5.554760000000000	14.228790000000000	7.831460000000000
H	5.481060000000000	14.169000000000000	14.257669999999999
H	5.268540000000000	7.812700000000000	7.773920000000000
H	5.218410000000000	7.754110000000000	14.194770000000000
H	8.697749999999999	12.254490000000001	11.533280000000000
H	9.574030000000000	12.863270000000000	9.687960000000000
H	9.285840000000000	10.046910000000000	13.147600000000001
H	9.185900000000000	9.517340000000001	14.586320000000001
H	8.841240000000001	14.164210000000001	10.143490000000000
H	8.729740000000000	10.908670000000001	9.394050000000000
H	10.135470000000000	10.622590000000001	8.793480000000001

Transition Metal: Cu; Functional Group: F; Adsorbate: OH

C	8.963800000000001	15.270910000000001	8.177840000000000
C	8.924239999999999	13.889670000000001	8.598229999999999
C	8.903290000000000	13.435169999999999	9.924090000000000
C	8.657610000000000	6.745750000000000	6.804990000000000
C	8.724620000000000	8.126609999999999	6.386020000000000
C	8.746930000000001	8.579910000000000	5.059910000000000
C	8.664370000000000	6.744490000000000	8.176589999999999
C	8.734740000000000	8.125159999999999	8.597860000000001
C	8.958200000000000	15.271690000000000	6.806150000000000
C	8.760289999999999	8.579520000000000	9.923480000000000
C	8.799620000000001	11.692769999999999	3.216310000000000
C	8.914949999999999	13.890739999999999	6.384080000000000
C	8.816060000000000	12.113870000000000	4.599380000000000
C	8.770140000000000	10.321800000000000	3.218300000000000
C	8.760899999999999	9.903960000000000	4.601480000000000
C	8.884420000000000	13.435510000000001	5.058520000000000
C	8.811959999999999	11.693669999999999	11.765910000000000
C	8.834700000000000	12.113049999999999	10.382690000000000
C	8.785180000000000	10.322920000000000	11.765990000000000
C	8.780810000000001	9.902939999999999	10.383039999999999
F	8.797180000000001	12.486079999999999	2.130930000000000
F	8.741669999999999	9.527139999999999	2.135840000000000
F	8.968130000000000	16.355360000000001	6.010470000000000
F	8.977490000000000	16.353349999999999	8.973269999999999
F	8.799429999999999	12.487830000000001	12.849650000000000
F	8.574830000000000	5.666220000000000	6.009440000000000
F	8.588050000000001	5.662990000000000	8.971990000000000
F	8.932969999999999	14.396000000000001	4.100170000000000
F	8.951449999999999	14.394240000000000	10.881290000000000
F	8.744320000000000	7.621040000000000	4.105020000000000
F	8.755599999999999	7.617890000000000	10.880960000000000
F	8.751659999999999	9.528330000000000	12.849050000000000
H	11.480680000000000	11.836600000000001	7.243060000000000
H	13.557720000000000	14.113450000000000	8.486990000000000
H	12.061900000000000	10.845140000000001	8.959220000000000
H	13.353579999999999	10.411009999999999	9.744260000000001
H	12.878819999999999	12.840630000000001	9.070010000000000
H	11.759470000000000	9.741970000000000	6.253570000000000
H	12.895230000000000	9.129189999999999	5.368850000000000
O	11.156520000000000	10.939299999999999	7.459080000000000
O	12.613580000000001	11.041370000000001	9.775309999999999
O	11.962230000000000	9.007640000000000	5.611570000000000
O	12.716699999999999	13.625750000000000	8.492900000000001
N	8.884119999999999	13.061769999999999	7.491490000000000
N	8.753959999999999	8.954269999999999	7.491610000000000
N	8.766510000000000	11.008740000000000	5.429100000000000
N	8.790060000000000	11.008039999999999	9.553850000000001
Cu	9.113989999999999	10.997640000000001	7.491580000000000

Transition Metal: Cu; Functional Group: F; Adsorbate: OOH

C	8.501590000000000	15.243090000000000	8.222780000000000
C	8.516200000000000	13.862930000000000	8.646879999999999
C	8.542289999999999	13.415270000000000	9.970310000000000
C	8.393850000000000	6.723340000000000	6.858270000000000
C	8.411780000000000	8.103690000000000	6.433320000000000
C	8.397140000000000	8.549709999999999	5.109090000000000
C	8.414920000000000	6.724200000000000	8.228310000000000
C	8.450089999999999	8.104850000000001	8.650300000000000
C	8.447850000000001	15.243140000000000	6.852940000000000
C	8.488680000000000	8.551250000000000	9.973509999999999
C	8.384069999999999	11.666079999999999	3.278200000000000
C	8.442190000000000	13.862909999999999	6.428740000000000
C	8.403150000000000	12.090579999999999	4.658290000000000
C	8.383490000000000	10.296450000000000	3.278930000000000
C	8.400820000000000	9.872270000000000	4.659640000000000
C	8.409770000000000	13.413860000000000	5.105660000000000
C	8.557169999999999	11.668979999999999	11.798819999999999
C	8.533640000000000	12.092150000000000	10.418150000000001
C	8.544129999999999	10.299440000000001	11.799650000000000
C	8.509190000000000	9.874779999999999	10.419820000000000
F	8.558160000000001	9.508419999999999	12.886220000000000
F	8.368470000000000	12.459099999999999	2.191210000000000
F	8.365840000000000	9.505240000000001	2.191780000000000
F	8.403390000000000	16.330150000000000	6.058240000000000
F	8.530640000000000	16.330190000000002	9.015980000000001
F	8.583180000000000	12.462569999999999	12.885059999999999
F	8.357260000000000	5.637570000000000	6.063740000000000
F	8.395429999999999	5.640600000000000	9.024690000000000
F	8.386350000000000	14.380350000000000	4.141000000000000
F	8.572850000000001	14.381320000000001	10.932630000000000
F	8.372700000000000	7.584290000000000	4.146260000000000
F	8.508260000000000	7.589020000000000	10.934160000000000
H	13.142360000000000	12.638620000000000	5.603750000000000
H	12.249630000000000	9.650230000000001	9.597560000000000
H	12.794969999999999	8.665850000000001	10.657080000000001
H	12.663010000000000	14.133020000000000	5.758870000000000
H	12.649860000000000	10.691879999999999	6.254600000000000
H	13.466600000000000	10.247980000000000	4.999410000000000
H	12.830769999999999	12.906020000000000	7.634280000000000
O	12.409649999999999	11.134729999999999	8.179390000000000
O	12.074500000000000	8.781240000000000	10.014239999999999
O	12.788209999999999	10.878830000000001	5.296610000000000
O	13.232150000000001	13.455810000000000	6.164090000000000
O	12.624040000000001	12.422960000000000	8.527900000000001
N	8.484180000000000	13.030799999999999	7.537900000000000
N	8.443740000000000	8.936340000000000	7.541410000000000
N	8.412080000000000	10.981740000000000	5.491450000000000
N	8.499790000000001	10.982550000000000	9.587190000000000
Cu	8.465280000000000	10.981619999999999	7.540730000000000

Transition Metal: Cu; Functional Group: H; Adsorbate: OH

Cu	5.539480000000000	10.984780000000001	11.002500000000000
H	5.279770000000000	12.351680000000000	5.886300000000000
H	5.180090000000000	9.631910000000000	5.893140000000000
H	5.473470000000000	16.103210000000001	9.634720000000000
H	5.451920000000000	16.107679999999998	12.355200000000000
H	5.255820000000000	12.362340000000000	16.112919999999999
H	5.129940000000000	5.890790000000000	9.644259999999999
H	5.139330000000000	5.891840000000000	12.366410000000000
H	5.407820000000000	14.198440000000000	7.789600000000000
H	5.370970000000000	14.205050000000000	14.205800000000000
H	5.177690000000000	7.790460000000000	7.799210000000000
H	5.191820000000000	7.796430000000000	14.210340000000000
H	5.181080000000000	9.642450000000000	16.112980000000000
H	7.875330000000000	11.834669999999999	10.720599999999999
H	9.414330000000000	14.225429999999999	12.104179999999999
H	8.536720000000001	10.884639999999999	12.435280000000001
H	9.869180000000000	10.369730000000001	13.081120000000000
H	9.653850000000000	12.700379999999999	12.249980000000001
H	8.451779999999999	9.765990000000000	9.852770000000000
H	9.791800000000000	9.539680000000001	9.100030000000000
C	5.433450000000000	15.252340000000000	11.682219999999999
C	5.385560000000000	13.866420000000000	12.103840000000000
C	5.350380000000000	13.432610000000000	13.434310000000000
C	5.156140000000000	6.743190000000000	10.320390000000000
C	5.194330000000000	8.130559999999999	9.900050000000000
C	5.193900000000000	8.563910000000000	8.570100000000000
C	5.161960000000000	6.743930000000000	11.690110000000001
C	5.203310000000000	8.131869999999999	12.108440000000000
C	5.443240000000000	15.250990000000000	10.311270000000000
C	5.210000000000000	8.568030000000000	13.437740000000000
C	5.265860000000000	11.678369999999999	6.741200000000000
C	5.397710000000000	13.864520000000001	9.892600000000000
C	5.300110000000000	12.099660000000000	8.128970000000001
C	5.214900000000000	10.309460000000000	6.744280000000000
C	5.219000000000000	9.892700000000000	8.133229999999999
C	5.370880000000000	13.427740000000000	8.562540000000000
C	5.251980000000000	11.687430000000001	15.259350000000000
C	5.290670000000000	12.105020000000000	13.870900000000001
C	5.215600000000000	10.318230000000000	15.260170000000000
C	5.230110000000000	9.897869999999999	13.872430000000000
O	7.583450000000000	10.937279999999999	10.981479999999999
O	9.202330000000000	11.072699999999999	13.165200000000000
O	8.944699999999999	9.105630000000000	9.297580000000000
O	9.688580000000000	13.442670000000000	11.597160000000001
N	5.357150000000000	13.037509999999999	10.998810000000001
N	5.214270000000000	8.959490000000001	11.003840000000000
N	5.252240000000000	10.997280000000000	8.959860000000001
N	5.258660000000000	11.000330000000000	13.043200000000001

Transition Metal: Cu; Functional Group: H; Adsorbate: OOH

H	5.002110000000000	9.626139999999999	16.079370000000001
H	4.952870000000000	12.360770000000000	5.871650000000000
H	4.944840000000000	9.638690000000000	5.870450000000000
H	4.991710000000000	16.104930000000000	9.624480000000000
H	5.004260000000000	16.098649999999999	12.345560000000001
H	4.999120000000000	12.347709999999999	16.084940000000000
H	4.974120000000000	5.890900000000000	9.611050000000001
H	4.996120000000000	5.889380000000000	12.333620000000000
H	4.972630000000000	14.207850000000001	7.770730000000000
H	5.000170000000000	14.198130000000001	14.190619999999999
H	4.956740000000000	7.790290000000000	7.765240000000000
H	5.004330000000000	7.783570000000000	14.181419999999999
H	9.635540000000001	12.587569999999999	9.247339999999999
H	8.961110000000000	9.536370000000000	13.178500000000000
H	9.999150000000000	8.998150000000001	14.178500000000000
H	8.873780000000000	13.947419999999999	9.426640000000001
H	9.157650000000000	10.623580000000000	9.818550000000000
H	10.197030000000000	10.230420000000001	8.724970000000001
H	9.267810000000001	12.777300000000000	11.266790000000000
C	5.001630000000000	15.246370000000001	11.668690000000000
C	4.996270000000000	13.858850000000000	12.086550000000001
C	4.992560000000000	13.427250000000001	13.416779999999999
C	4.974390000000000	6.743550000000000	10.287760000000000
C	4.967680000000000	8.131370000000000	9.868320000000001
C	4.960600000000000	8.561750000000000	8.538500000000001
C	4.983700000000000	6.742160000000000	11.657570000000000
C	4.980230000000000	8.129280000000000	12.079810000000000
C	4.997010000000000	15.249169999999999	10.297530000000000
C	4.985080000000000	8.556179999999999	13.410530000000000
C	4.957160000000000	11.684749999999999	6.724730000000000
C	4.989380000000000	13.862700000000000	9.874050000000000
C	4.968980000000000	12.104279999999999	8.112200000000000
C	4.952630000000000	10.314520000000000	6.723770000000000
C	4.961240000000000	9.892899999999999	8.110780000000000
C	4.978890000000000	13.434620000000001	8.542380000000000
C	4.990450000000000	11.673140000000000	15.230610000000000
C	4.983930000000000	12.096349999999999	13.843050000000000
C	4.990660000000000	10.303710000000001	15.228000000000000
C	4.982040000000000	9.885640000000000	13.840190000000000
O	8.806690000000000	10.994840000000000	11.737550000000001
O	9.197469999999999	8.736760000000000	13.694089999999999
O	9.442090000000000	10.820100000000000	8.894539999999999
O	9.604699999999999	13.419350000000000	9.794240000000000
O	9.105520000000000	12.251820000000000	12.142730000000000
Cu	4.981220000000000	10.993610000000000	10.978500000000000
N	4.990250000000000	13.030440000000000	10.979010000000001
N	4.971080000000000	8.960770000000000	10.974750000000000
N	4.969820000000000	10.997940000000000	8.942200000000000
N	4.975570000000000	10.992000000000001	13.011010000000001

Transition Metal: Fe; Functional Group: F; Adsorbate: OH

C	8.838480000000001	15.290240000000001	8.191710000000000
C	8.758390000000000	13.915680000000000	8.618610000000000
C	8.704630000000000	13.458800000000000	9.942959999999999
C	8.671659999999999	6.747380000000000	6.815160000000000
C	8.630710000000001	8.124840000000001	6.390740000000000
C	8.582269999999999	8.585380000000001	5.066820000000000
C	8.701029999999999	6.746490000000000	8.190099999999999
C	8.677680000000001	8.123630000000000	8.617310000000000
C	8.841749999999999	15.289859999999999	6.816930000000000
C	8.669710000000000	8.584490000000001	9.942349999999999
C	8.570660000000000	11.707409999999999	3.230170000000000
C	8.763150000000000	13.914650000000000	6.390830000000000
C	8.629410000000000	12.133250000000000	4.608380000000000
C	8.535840000000000	10.334860000000001	3.231890000000000
C	8.568840000000000	9.910410000000001	4.610840000000000
C	8.710990000000001	13.456270000000000	5.066410000000000
C	8.577610000000000	11.708280000000000	11.779930000000000
C	8.635710000000000	12.134940000000000	10.401710000000000
C	8.576160000000000	10.334410000000000	11.779190000000000
C	8.628489999999999	9.908820000000000	10.401199999999999
F	8.523910000000001	9.546410000000000	12.867459999999999
F	8.550219999999999	12.494800000000000	2.140560000000000
F	8.485900000000001	9.547129999999999	2.144780000000000
F	8.908210000000000	16.376639999999998	6.028400000000000
F	8.901140000000000	16.377520000000001	8.978809999999999
F	8.527350000000000	12.494780000000000	12.868910000000000
F	8.686070000000001	5.658270000000000	6.027620000000000
F	8.741250000000001	5.656740000000000	8.977200000000000
F	8.738899999999999	14.420790000000000	4.103310000000000
F	8.722350000000000	14.422720000000000	10.906490000000000
F	8.552020000000001	7.623640000000000	4.104410000000000
F	8.703810000000001	7.621450000000000	10.907579999999999
H	11.522080000000001	11.823950000000000	7.518540000000000
H	13.421980000000000	13.274730000000000	7.151080000000000
H	12.551930000000000	10.358129999999999	8.756560000000000
H	13.406680000000000	10.288060000000000	10.057930000000001
H	13.313650000000001	12.419260000000000	8.444599999999999
H	11.894850000000000	10.110620000000001	5.968660000000000
H	13.076610000000001	9.314769999999999	5.361760000000000
O	11.031040000000001	10.959490000000001	7.498220000000000
O	13.437080000000000	10.572530000000000	9.128520000000000
O	12.245189999999999	9.757360000000000	5.119720000000000
O	12.831000000000000	13.085360000000000	7.901000000000000
N	8.727100000000000	13.086639999999999	7.505220000000000
N	8.642379999999999	8.951860000000000	7.504580000000000
N	8.617960000000000	11.022080000000001	5.437750000000000
N	8.653400000000000	11.022340000000000	9.574540000000001
Fe	9.161840000000000	11.011939999999999	7.500400000000000

Transition Metal: Fe; Functional Group: F; Adsorbate: OOH

C	8.765140000000001	15.238400000000000	8.224550000000001
C	8.683920000000001	13.861079999999999	8.640340000000000
C	8.614160000000000	13.421980000000000	9.959660000000000
C	8.496900000000000	6.764290000000000	6.827040000000000
C	8.545710000000000	8.143050000000001	6.410870000000000
C	8.563230000000001	8.583330000000000	5.090360000000000
C	8.541440000000000	6.759920000000000	8.195040000000001
C	8.601279999999999	8.137079999999999	8.618600000000001
C	8.862550000000001	15.236990000000000	6.858380000000000
C	8.625900000000000	8.570840000000000	9.941380000000001
C	8.755720000000000	11.692959999999999	3.285490000000000
C	8.831390000000001	13.859650000000000	6.433820000000000
C	8.795349999999999	12.107820000000000	4.666580000000000
C	8.650080000000001	10.329040000000001	3.280380000000000
C	8.630720000000000	9.904480000000000	4.658520000000000
C	8.881560000000000	13.423560000000000	5.111460000000000
C	8.560250000000000	11.675000000000001	11.769560000000000
C	8.587580000000001	12.099980000000000	10.392230000000000
C	8.580159999999999	10.307090000000001	11.763470000000000
C	8.615500000000001	9.891760000000000	10.381830000000001
F	8.789529999999999	12.491910000000001	2.204850000000000
F	8.560660000000000	9.540210000000000	2.195150000000000
F	8.956200000000001	16.320110000000000	6.065240000000000
F	8.744780000000000	16.322050000000001	9.021520000000001
F	8.516550000000001	12.465820000000001	12.856430000000000
F	8.403860000000000	5.686260000000000	6.027930000000000
F	8.516100000000000	5.676140000000000	8.989319999999999
F	8.998530000000001	14.386649999999999	4.155290000000000
F	8.585860000000000	14.383459999999999	10.922580000000000
F	8.521580000000000	7.625210000000000	4.124310000000000
F	8.625030000000001	7.606450000000000	10.900100000000000
F	8.554520000000000	9.506910000000000	12.842770000000000
H	13.263330000000000	12.247190000000000	6.255990000000000
H	12.418930000000000	10.138830000000000	9.343260000000001
H	13.323969999999999	9.388850000000000	10.347780000000000
H	12.943170000000000	13.783230000000000	6.279760000000000
H	12.229290000000001	10.298090000000000	6.134110000000000
H	13.679580000000000	9.860930000000000	5.826630000000000
H	11.952560000000000	12.306740000000000	7.925930000000000
O	10.677289999999999	10.912419999999999	7.509080000000000
O	12.826470000000000	9.265590000000000	9.521490000000000
O	13.006620000000000	10.520849999999999	5.581400000000000
O	13.139350000000000	13.025539999999999	6.856950000000000
O	11.390750000000001	11.714729999999999	8.519310000000001
N	8.711449999999999	13.015480000000000	7.533870000000000
N	8.593430000000000	8.987450000000001	7.517250000000000
N	8.705040000000000	11.004490000000001	5.510420000000000
N	8.610659999999999	10.999269999999999	9.540559999999999
Fe	8.902189999999999	11.003430000000000	7.535010000000000

Transition Metal: Fe; Functional Group: H; Adsorbate: OH

Fe	5.684970000000000	11.003340000000000	10.989319999999999
H	5.265740000000000	12.378180000000000	5.909450000000000
H	5.197800000000000	9.652240000000001	5.910550000000000
H	5.503880000000000	16.094180000000001	9.632610000000000
H	5.511930000000000	16.091490000000000	12.358549999999999
H	5.331180000000000	12.371270000000001	16.077529999999999
H	5.277250000000000	5.932800000000000	9.623900000000001
H	5.305010000000000	5.928320000000000	12.350750000000000
H	5.429300000000000	14.217990000000000	7.786570000000000
H	5.457320000000000	14.211630000000000	14.200939999999999
H	5.276270000000000	7.810500000000000	7.786400000000000
H	5.334370000000000	7.803870000000000	14.195050000000000
H	5.279720000000000	9.645580000000001	16.076380000000000
H	8.020379999999999	11.833660000000000	10.773930000000000
H	9.305260000000001	14.189950000000000	12.030040000000000
H	8.622859999999999	10.828310000000000	12.502700000000001
H	9.951219999999999	10.374720000000000	13.184040000000000
H	9.651640000000000	12.698330000000000	12.287350000000000
H	8.533810000000001	9.733440000000000	9.826960000000000
H	9.819950000000000	9.526820000000001	8.990950000000000
C	5.500700000000000	15.240539999999999	11.680400000000001
C	5.475450000000000	13.859330000000000	12.098670000000000
C	5.446660000000000	13.441140000000001	13.427780000000000
C	5.305210000000000	6.782530000000000	10.303290000000001
C	5.333180000000000	8.164400000000001	9.885429999999999
C	5.301900000000000	8.582229999999999	8.557140000000000
C	5.320680000000000	6.780370000000000	11.673539999999999
C	5.358070000000000	8.161490000000001	12.094709999999999
C	5.495500000000000	15.242030000000000	10.309070000000000
C	5.352070000000000	8.576860000000000	13.425050000000001
C	5.284890000000000	11.699949999999999	6.760060000000000
C	5.465360000000000	13.861800000000001	9.887829999999999
C	5.356700000000000	12.117649999999999	8.142099999999999
C	5.249460000000000	10.330760000000000	6.759960000000000
C	5.300880000000000	9.911030000000000	8.141410000000000
C	5.422390000000000	13.445959999999999	8.558260000000001
C	5.341710000000000	11.693550000000000	15.226160000000000
C	5.392550000000000	12.112380000000000	13.843570000000000
C	5.315970000000000	10.324299999999999	15.226080000000000
C	5.350970000000000	9.905530000000001	13.843370000000000
O	7.630650000000000	10.957509999999999	10.978170000000000
O	9.256970000000001	11.053540000000000	13.239300000000000
O	8.993589999999999	9.081020000000001	9.242260000000000
O	9.629120000000000	13.390050000000000	11.582150000000000
N	5.460540000000000	13.020519999999999	10.992369999999999
N	5.371720000000000	9.001920000000000	10.991149999999999
N	5.356550000000000	11.013510000000000	8.980240000000000
N	5.387560000000000	11.008620000000001	13.004750000000000

Transition Metal: Fe; Functional Group: H; Adsorbate: OOH

H	5.371280000000000	12.420050000000000	5.952410000000000
H	5.180330000000000	9.701180000000001	5.917620000000000
H	5.432270000000000	16.095350000000000	9.710410000000000
H	5.274220000000000	16.072659999999999	12.431710000000001
H	5.055880000000000	12.316459999999999	16.109470000000002
H	5.016000000000000	5.937650000000000	9.602679999999999
H	5.076940000000000	5.914510000000000	12.328550000000000
H	5.505240000000000	14.231500000000000	7.854150000000000
H	5.171300000000000	14.175860000000000	14.253840000000000
H	5.111890000000000	7.838170000000000	7.776460000000000
H	5.181150000000000	7.773670000000000	14.181839999999999
H	5.086450000000000	9.588469999999999	16.077660000000002
H	9.779010000000000	12.298959999999999	9.772309999999999
H	8.962890000000000	10.008730000000000	12.963609999999999
H	9.894909999999999	9.546830000000000	14.100090000000000
H	9.303839999999999	13.787190000000001	9.822430000000001
H	8.675850000000001	10.431340000000001	9.625000000000000
H	10.119360000000000	9.905870000000000	9.446899999999999
H	8.541740000000001	12.247500000000000	11.498350000000000
C	5.314070000000000	15.227570000000000	11.747470000000000
C	5.277140000000000	13.841460000000000	12.152410000000000
C	5.202630000000000	13.411870000000000	13.474480000000000
C	5.076740000000000	6.781590000000000	10.286970000000000
C	5.139460000000000	8.168170000000000	9.881390000000000
C	5.158260000000000	8.599449999999999	8.557370000000001
C	5.104720000000000	6.769500000000000	11.655550000000000
C	5.174730000000000	8.148050000000000	12.085750000000001
C	5.396270000000000	15.237900000000000	10.379940000000000
C	5.191010000000000	8.552899999999999	13.417579999999999
C	5.341160000000000	11.730900000000000	6.794070000000000
C	5.405840000000000	13.857650000000000	9.949460000000000
C	5.385550000000000	12.130590000000000	8.183299999999999
C	5.244450000000000	10.365990000000000	6.776700000000000
C	5.234720000000000	9.930410000000000	8.156060000000000
C	5.451450000000000	13.451980000000001	8.616940000000000
C	5.107070000000000	11.646269999999999	15.253520000000000
C	5.170120000000000	12.079800000000001	13.875230000000000
C	5.121570000000000	10.278169999999999	15.236720000000000
C	5.184590000000000	9.876690000000000	13.848269999999999
Fe	5.498910000000000	11.001680000000000	11.027480000000001
O	7.268650000000000	10.866759999999999	11.008290000000001
O	9.444680000000000	9.223380000000001	13.301390000000000
O	9.495839999999999	10.568400000000000	9.099890000000000
O	9.685730000000000	13.082079999999999	10.373150000000001
O	8.011640000000000	11.608639999999999	12.062939999999999
N	5.325090000000000	13.005300000000000	11.043250000000000
N	5.186570000000000	9.001890000000000	10.991339999999999
N	5.314540000000000	11.020410000000000	9.015029999999999
N	5.206410000000000	10.988099999999999	13.018500000000000

Transition Metal: Mn; Functional Group: F; Adsorbate: OH

C	8.741289999999999	15.254949999999999	8.189900000000000
C	8.750430000000000	13.877739999999999	8.611510000000001
C	8.760330000000000	13.428979999999999	9.934910000000000
C	8.759610000000000	6.748540000000000	6.795060000000000
C	8.759449999999999	8.125800000000000	6.374260000000000
C	8.731719999999999	8.572550000000000	5.050820000000000
C	8.760600000000000	6.744030000000000	8.167540000000001
C	8.767670000000001	8.119030000000000	8.597550000000000
C	8.735600000000000	15.259690000000001	6.817030000000000
C	8.766220000000001	8.559650000000000	9.924060000000001
C	8.614300000000000	11.695560000000000	3.234060000000000
C	8.734780000000001	13.885040000000000	6.385850000000000
C	8.674830000000000	12.119680000000001	4.611360000000000
C	8.618230000000001	10.323600000000001	3.232460000000000
C	8.683790000000000	9.896810000000000	4.607920000000000
C	8.710839999999999	13.443040000000000	5.060090000000000
C	8.753610000000000	11.676480000000000	11.755850000000001
C	8.755470000000001	12.104419999999999	10.378760000000000
C	8.752840000000001	10.304770000000000	11.753259999999999
C	8.755670000000000	9.882220000000000	10.374350000000000
F	8.748609999999999	9.511540000000000	12.836180000000001
F	8.551660000000000	12.488280000000000	2.152150000000000
F	8.557150000000000	9.534060000000000	2.148620000000000
F	8.724340000000000	16.347290000000001	6.029430000000000
F	8.735830000000000	16.337450000000000	8.985160000000000
F	8.750100000000000	12.465960000000001	12.841450000000000
F	8.746980000000001	5.668140000000000	5.999850000000000
F	8.748720000000000	5.658230000000000	8.956750000000000
F	8.715520000000000	14.408149999999999	4.099620000000000
F	8.767980000000000	14.390660000000000	10.898420000000000
F	8.737310000000001	7.613310000000000	4.088480000000000
F	8.767239999999999	7.593580000000000	10.882460000000000
H	11.411310000000000	11.894629999999999	7.268320000000000
H	13.068110000000001	14.242310000000000	8.486450000000000
H	12.100820000000001	10.823380000000000	8.909660000000001
H	13.425850000000001	10.323729999999999	9.563620000000000
H	13.114960000000000	12.703110000000001	8.709980000000000
H	11.972400000000000	9.696750000000000	6.549000000000000
H	13.192700000000000	9.229810000000001	5.707320000000000
Mn	9.031050000000000	11.002050000000001	7.488960000000000
O	11.009090000000000	11.022169999999999	7.456680000000000
O	12.755330000000001	11.025160000000000	9.632560000000000
O	12.386110000000000	8.897959999999999	6.136710000000000
O	12.998580000000000	13.395049999999999	8.015330000000001
N	8.741199999999999	13.048430000000000	7.496130000000000
N	8.762330000000000	8.955570000000000	7.488200000000000
N	8.699740000000000	11.006940000000000	5.441170000000000
N	8.747900000000000	10.994999999999999	9.544230000000001

Transition Metal: Mn; Functional Group: F; Adsorbate: OOH

C	8.559490000000000	15.290780000000000	8.200310000000000
C	8.560499999999999	13.913810000000000	8.627570000000000
C	8.542280000000000	13.468990000000000	9.951440000000000
C	8.586580000000000	6.775300000000000	6.838540000000000
C	8.609970000000001	8.151719999999999	6.409690000000000
C	8.600270000000000	8.592860000000000	5.085060000000000
C	8.603050000000000	6.777620000000000	8.209590000000000
C	8.634480000000000	8.155270000000000	8.631000000000000
C	8.601789999999999	15.288550000000001	6.829020000000000
C	8.628370000000000	8.599480000000000	9.954160000000000
C	8.689990000000000	11.712130000000000	3.261090000000000
C	8.635199999999999	13.910900000000000	6.405630000000000
C	8.694810000000000	12.138660000000000	4.637310000000000
C	8.631069999999999	10.340800000000000	3.261290000000000
C	8.620080000000000	9.916169999999999	4.637850000000000
C	8.700150000000001	13.462529999999999	5.083790000000000
C	8.495419999999999	11.717730000000000	11.770980000000000
C	8.543889999999999	12.145189999999999	10.396170000000000
C	8.538620000000000	10.346030000000001	11.771680000000000
C	8.598229999999999	9.923510000000000	10.396680000000000
F	8.517410000000000	9.554290000000000	12.855520000000000
F	8.719310000000000	12.500769999999999	2.174660000000000
F	8.586160000000000	9.549620000000001	2.177430000000000
F	8.593810000000000	16.371469999999999	6.033070000000000
F	8.519430000000000	16.375959999999999	8.991320000000000
F	8.406120000000000	12.505080000000000	12.855150000000000
F	8.548800000000000	5.690830000000000	6.046700000000000
F	8.574930000000000	5.696880000000000	9.005789999999999
F	8.756700000000000	14.425120000000000	4.121170000000000
F	8.519940000000000	14.431350000000000	10.913959999999999
F	8.567030000000001	7.627860000000000	4.124880000000000
F	8.618819999999999	7.639630000000000	10.916110000000000
H	12.301010000000000	12.276220000000000	7.995800000000000
H	13.646570000000001	12.141280000000000	6.350000000000000
H	12.119289999999999	10.195250000000000	9.425459999999999
H	13.026669999999999	9.389709999999999	10.388520000000000
H	13.709429999999999	13.688040000000001	6.602650000000000
H	12.134760000000000	10.681550000000000	6.102330000000000
H	13.369830000000000	9.828040000000000	5.666840000000000
Mn	8.884219999999999	11.039009999999999	7.523380000000000
O	10.869890000000000	11.162739999999999	7.333440000000000
O	12.224720000000000	9.311710000000000	9.844880000000000
O	12.916150000000000	10.669750000000001	5.486740000000000
O	13.725640000000000	12.830460000000000	7.060990000000000
O	11.546849999999999	11.810610000000000	8.464630000000000
N	8.592110000000000	13.081180000000000	7.518160000000000
N	8.637269999999999	8.987900000000000	7.518450000000000
N	8.651240000000000	11.027189999999999	5.470270000000000
N	8.597429999999999	11.035280000000000	9.563290000000000

Transition Metal: Mn; Functional Group: H; Adsorbate: OH

H	5.262080000000000	9.618760000000000	16.086900000000000
H	5.136240000000000	12.372450000000001	5.896170000000000
H	5.146010000000000	9.647869999999999	5.891080000000000
H	5.208400000000000	16.100420000000000	9.646490000000000
H	5.243880000000000	16.089559999999999	12.369820000000001
H	5.264380000000000	12.342150000000000	16.093810000000001
H	5.219200000000000	5.905230000000000	9.611660000000001
H	5.245700000000000	5.893360000000000	12.336230000000000
H	5.217520000000000	14.217800000000000	7.789200000000000
H	5.306280000000000	14.194039999999999	14.211069999999999
H	5.233040000000000	7.798140000000000	7.773950000000000
H	5.300310000000000	7.775720000000000	14.191330000000001
H	7.974920000000000	11.825810000000001	10.653850000000000
H	9.447730000000000	14.210810000000000	12.022570000000000
H	8.611340000000000	10.884110000000000	12.374879999999999
H	9.946300000000001	10.356310000000001	12.994570000000000
H	9.708510000000000	12.689240000000000	12.175170000000000
H	8.508360000000000	9.635020000000001	10.039970000000000
H	9.788320000000001	9.323140000000000	9.221790000000000
C	5.264030000000000	15.239640000000000	11.690360000000000
C	5.304290000000000	13.856750000000000	12.107650000000000
C	5.313180000000000	13.425060000000000	13.436220000000000
C	5.245620000000000	6.754230000000000	10.291950000000000
C	5.270380000000000	8.137940000000000	9.874670000000000
C	5.247050000000000	8.567700000000000	8.547140000000001
C	5.260700000000000	6.748450000000000	11.662710000000001
C	5.296610000000000	8.129180000000000	12.091020000000000
C	5.244060000000000	15.245180000000000	10.318870000000000
C	5.306300000000000	8.550240000000001	13.422430000000000
C	5.173550000000000	11.693989999999999	6.746250000000000
C	5.270560000000000	13.865869999999999	9.889650000000000
C	5.226850000000000	12.114480000000000	8.128890000000000
C	5.178120000000000	10.323200000000000	6.743610000000000
C	5.232140000000000	9.897890000000000	8.124490000000000
C	5.242430000000000	13.443519999999999	8.558439999999999
C	5.280820000000000	11.667289999999999	15.240370000000000
C	5.307370000000000	12.093990000000000	13.858570000000000
C	5.280490000000000	10.297070000000000	15.236520000000001
C	5.305190000000000	9.878220000000001	13.852980000000001
Mn	5.578590000000000	10.993720000000000	10.986459999999999
O	7.584840000000000	10.977819999999999	10.943800000000000
O	9.287830000000000	11.065580000000001	13.093240000000000
O	9.003840000000000	8.893470000000001	9.602490000000000
O	9.727539999999999	13.428550000000000	11.518060000000000
N	5.309400000000000	13.029380000000000	10.995020000000000
N	5.302030000000000	8.965460000000000	10.986039999999999
N	5.257090000000000	11.004670000000001	8.957330000000001
N	5.316610000000000	10.988030000000000	13.024089999999999

Transition Metal: Mn; Functional Group: H; Adsorbate: OOH

H	5.077170000000000	9.538510000000000	16.109929999999999
H	5.274960000000000	12.369160000000001	5.947640000000000
H	5.208130000000000	9.647580000000000	5.917140000000000
H	5.235160000000000	16.069189999999999	9.721460000000000
H	5.147160000000000	16.041609999999999	12.443130000000000
H	5.048680000000000	12.262700000000001	16.139109999999999
H	5.124800000000000	5.870390000000000	9.617960000000000
H	5.128170000000000	5.844630000000000	12.341220000000000
H	5.318550000000000	14.195010000000000	7.855260000000000
H	5.122900000000000	14.131119999999999	14.272919999999999
H	5.198070000000000	7.776740000000000	7.787300000000000
H	5.175840000000000	7.713600000000000	14.204540000000000
H	8.759910000000000	12.261469999999999	11.609850000000000
H	9.958520000000000	12.427009999999999	9.862539999999999
H	8.970370000000001	10.028879999999999	12.957879999999999
H	9.889469999999999	9.549189999999999	14.101810000000000
H	9.432040000000001	13.891080000000001	9.980200000000000
H	8.760330000000000	10.711830000000001	9.734650000000000
H	10.135310000000000	10.045339999999999	9.409640000000000
C	5.184380000000000	15.196090000000000	11.759290000000000
C	5.188750000000000	13.809040000000000	12.168630000000000
C	5.149790000000000	13.368230000000001	13.492979999999999
C	5.156540000000000	6.715310000000000	10.302619999999999
C	5.200270000000000	8.101900000000001	9.892640000000000
C	5.213470000000000	8.540360000000000	8.567140000000000
C	5.155950000000000	6.702220000000000	11.672560000000001
C	5.194850000000000	8.080510000000000	12.108010000000000
C	5.230110000000000	15.209780000000000	10.389030000000000
C	5.182890000000000	8.493050000000000	13.440930000000000
C	5.269310000000000	11.683900000000000	6.793190000000000
C	5.261780000000000	13.830830000000001	9.953400000000000
C	5.289360000000000	12.090800000000000	8.179970000000001
C	5.235380000000000	10.313330000000001	6.777700000000000
C	5.238470000000000	9.874520000000000	8.155010000000001
C	5.299340000000000	13.416380000000000	8.619970000000000
C	5.089080000000000	11.595820000000000	15.280040000000000
C	5.142060000000000	12.033709999999999	13.903280000000001
C	5.105270000000000	10.225030000000000	15.265860000000000
C	5.163540000000000	9.818059999999999	13.880240000000001
Mn	5.485650000000000	10.955909999999999	11.039280000000000
O	7.496230000000000	10.972619999999999	10.930690000000000
O	9.354979999999999	9.216749999999999	13.361010000000000
O	9.558350000000001	10.778180000000001	9.131840000000000
O	9.907560000000000	13.205180000000000	10.479830000000000
O	8.158140000000000	11.619930000000000	12.081340000000001
N	5.231630000000000	12.989150000000000	11.053520000000001
N	5.221020000000000	8.922950000000000	11.007720000000001
N	5.269410000000000	10.972320000000000	8.999510000000001
N	5.181600000000000	10.935269999999999	13.060480000000000

Transition Metal: Ni; Functional Group: F; Adsorbate: OH

Ni	9.043540000000000	10.995490000000000	7.490100000000000
C	8.773080000000000	15.288330000000000	8.184010000000001
C	8.805360000000000	13.904570000000000	8.597510000000000
C	8.790990000000001	13.432029999999999	9.913069999999999
C	8.769880000000001	6.713220000000000	6.799330000000000
C	8.805339999999999	8.097820000000000	6.386740000000000
C	8.792040000000000	8.567349999999999	5.070840000000000
C	8.794680000000000	6.710230000000000	8.169499999999999
C	8.845649999999999	8.093260000000001	8.587310000000000
C	8.792970000000000	15.291869999999999	6.813150000000000
C	8.865330000000000	8.559250000000000	9.904940000000000
C	8.833800000000000	11.690189999999999	3.265350000000000
C	8.838279999999999	13.909970000000000	6.394530000000000
C	8.820209999999999	12.113030000000000	4.645280000000000
C	8.813120000000000	10.321910000000001	3.264760000000000
C	8.786379999999999	9.898820000000001	4.644200000000000
C	8.856380000000000	13.442040000000000	5.076840000000000
C	8.816649999999999	11.677479999999999	11.720140000000001
C	8.789820000000001	12.101599999999999	10.340809999999999
C	8.838480000000001	10.309510000000000	11.718990000000000
C	8.827140000000000	9.888090000000000	10.338410000000000
F	8.832610000000001	9.516380000000000	12.802860000000001
F	8.829850000000000	12.483409999999999	2.180950000000000
F	8.792930000000000	9.531120000000000	2.180120000000000
F	8.761270000000000	16.372930000000000	6.014240000000000
F	8.729160000000000	16.366409999999998	8.986540000000000
F	8.798310000000001	12.468650000000000	12.805320000000000
F	8.716340000000001	5.637330000000000	5.996620000000000
F	8.760230000000000	5.630980000000000	8.970330000000001
F	8.910100000000000	14.389379999999999	4.105710000000000
F	8.777500000000000	14.377219999999999	10.887380000000000
F	8.776949999999999	7.624520000000000	4.098500000000000
F	8.916029999999999	7.611430000000000	10.874900000000000
H	11.288340000000000	11.923080000000001	7.321150000000000
H	13.092140000000001	14.272480000000000	8.545240000000000
H	11.991580000000001	10.850890000000000	8.959149999999999
H	13.316300000000000	10.360920000000000	9.636749999999999
H	13.000690000000001	12.738910000000001	8.803920000000000
H	11.857849999999999	9.846299999999999	6.338920000000000
H	13.119009999999999	9.445740000000001	5.515440000000000
O	11.001530000000001	11.000330000000000	7.484330000000000
O	12.627470000000001	11.044200000000000	9.705819999999999
O	12.233980000000001	9.130190000000001	5.764720000000000
O	12.872479999999999	13.430870000000001	8.112050000000000
N	8.853790000000000	13.076040000000001	7.494750000000000
N	8.857699999999999	8.926360000000001	7.487620000000000
N	8.747579999999999	11.004740000000000	5.486450000000000
N	8.754080000000000	10.994300000000001	9.497760000000000

Transition Metal: Ni; Functional Group: F; Adsorbate: OOH

Ni	8.849270000000001	11.056990000000001	7.527150000000000
C	8.506140000000000	15.305370000000000	8.225500000000000
C	8.496600000000001	13.923930000000000	8.649100000000001
C	8.515430000000000	13.466780000000000	9.972700000000000
C	8.453300000000000	6.770980000000000	6.854220000000000
C	8.457739999999999	8.152839999999999	6.431310000000000
C	8.412720000000000	8.606629999999999	5.105260000000000
C	8.538729999999999	6.770940000000000	8.223319999999999
C	8.585070000000000	8.152740000000000	8.642530000000001
C	8.513809999999999	15.304950000000000	6.853660000000000
C	8.640050000000000	8.607020000000000	9.966770000000000
C	8.472260000000000	11.719420000000000	3.258780000000000
C	8.507830000000000	13.923000000000000	6.430040000000000
C	8.508740000000000	12.142799999999999	4.641610000000000
C	8.414370000000000	10.349610000000000	3.260990000000000
C	8.433690000000000	9.928039999999999	4.643480000000000
C	8.528010000000000	13.465520000000000	5.104600000000000
C	8.554990000000000	11.719070000000000	11.814380000000000
C	8.541069999999999	12.142630000000000	10.432600000000001
C	8.594600000000000	10.347960000000000	11.811450000000001
C	8.607860000000001	9.929830000000001	10.427650000000000
F	8.595020000000000	9.552450000000000	12.896940000000001
F	8.488560000000000	12.509539999999999	2.169180000000000
F	8.351620000000000	9.556490000000000	2.175250000000000
F	8.522580000000000	16.392740000000000	6.059520000000000
F	8.508290000000001	16.393200000000000	9.019530000000000
F	8.522280000000000	12.507040000000000	12.904880000000000
F	8.369120000000001	5.684060000000000	6.063440000000000
F	8.551589999999999	5.684360000000000	9.016750000000000
F	8.556260000000000	14.432000000000000	4.143650000000000
F	8.524440000000000	14.431490000000000	10.934540000000000
F	8.355630000000000	7.639810000000000	4.146550000000000
F	8.713530000000000	7.643860000000000	10.924750000000000
H	13.530030000000000	11.986890000000001	6.161060000000000
H	12.285159999999999	10.145670000000001	9.399250000000000
H	13.180830000000000	9.249020000000000	10.275910000000000
H	13.587300000000001	13.527620000000001	6.467900000000000
H	12.021490000000000	10.495860000000000	5.782010000000000
H	13.276820000000001	9.744059999999999	5.265820000000000
H	12.279100000000000	12.255409999999999	7.776010000000000
O	10.750999999999999	11.195340000000000	7.321390000000000
O	12.580220000000001	9.222420000000000	9.511300000000000
O	12.813129999999999	10.598459999999999	5.211420000000000
O	13.611540000000000	12.653150000000000	6.894780000000000
O	11.437329999999999	11.963360000000000	8.285750000000000
N	8.487270000000001	13.094030000000000	7.539000000000000
N	8.530070000000000	8.984660000000000	7.536450000000000
N	8.489480000000000	11.036130000000000	5.472720000000000
N	8.566290000000000	11.038169999999999	9.600759999999999

Transition Metal: Ni; Functional Group: H; Adsorbate: OH

Ni	5.456730000000000	10.993860000000000	10.969030000000000
C	5.319680000000000	15.210380000000001	11.665950000000000
C	5.315810000000000	13.826950000000000	12.080000000000000
C	5.297900000000000	13.415160000000000	13.406180000000001
C	5.265430000000000	6.780040000000000	10.275240000000000
C	5.268480000000000	8.164930000000000	9.862130000000001
C	5.244350000000000	8.575020000000000	8.536410000000000
C	5.304040000000000	6.775000000000000	11.641280000000000
C	5.326460000000000	8.157280000000000	12.063520000000000
C	5.344870000000000	15.215700000000000	10.298130000000000
C	5.348780000000000	8.559410000000000	13.392460000000000
C	5.276920000000000	11.689800000000000	6.752010000000000
C	5.349130000000000	13.835430000000001	9.874470000000001
C	5.306040000000000	12.105250000000000	8.135980000000000
C	5.237390000000000	10.323430000000000	6.750900000000000
C	5.247960000000000	9.903330000000000	8.133050000000001
C	5.349580000000000	13.431120000000000	8.545610000000000
C	5.284130000000000	11.666040000000001	15.192130000000001
C	5.292530000000000	12.087230000000000	13.809860000000000
C	5.307990000000000	10.299580000000001	15.188380000000000
C	5.325490000000000	9.885479999999999	13.803879999999999
N	5.326850000000000	12.989710000000001	10.974230000000000
N	5.295300000000000	9.002070000000000	10.965880000000000
N	5.272540000000000	11.002900000000000	8.975730000000000
N	5.299800000000000	10.988250000000001	12.965859999999999
O	7.505860000000000	10.949719999999999	10.948630000000000
O	9.121140000000000	11.087660000000000	13.125330000000000
O	8.864570000000001	9.122360000000000	9.252730000000000
O	9.609059999999999	13.459580000000001	11.558610000000000
H	5.310820000000000	9.614390000000000	16.033650000000002
H	5.282640000000000	12.373799999999999	5.906000000000000
H	5.209070000000000	9.641590000000001	5.903460000000000
H	5.351170000000000	16.065890000000000	9.619320000000000
H	5.300330000000000	16.055499999999999	12.350989999999999
H	5.264940000000000	12.346550000000001	16.040610000000001
H	5.240550000000000	5.936220000000000	9.589040000000001
H	5.312170000000000	5.926070000000000	12.321540000000001
H	5.375010000000000	14.203989999999999	7.776560000000000
H	5.290800000000000	14.184189999999999	14.179349999999999
H	5.237110000000000	7.805890000000000	7.762940000000000
H	5.373190000000000	7.785700000000000	14.161289999999999
H	7.784780000000000	11.849250000000000	10.680640000000000
H	9.332039999999999	14.242270000000000	12.063980000000001
H	8.457030000000000	10.900700000000001	12.392030000000000
H	9.789880000000000	10.386440000000000	13.043110000000000
H	9.572960000000000	12.716419999999999	12.210470000000001
H	8.374350000000000	9.781430000000000	9.812700000000000
H	9.714130000000001	9.554370000000000	9.060890000000001

Transition Metal: Ni; Functional Group: H; Adsorbate: OOH

Ni	5.191360000000000	11.005810000000000	10.989710000000001
C	5.080110000000000	15.220390000000000	11.681460000000000
C	5.079550000000000	13.835649999999999	12.094830000000000
C	5.053760000000000	13.426430000000000	13.421720000000001
C	5.022380000000000	6.789210000000000	10.296419999999999
C	5.021420000000000	8.174350000000000	9.882140000000000
C	4.994820000000000	8.583900000000000	8.555740000000000
C	5.087090000000000	6.787240000000000	11.661490000000001
C	5.114710000000000	8.170769999999999	12.079770000000000
C	5.122230000000000	15.224470000000000	10.314299999999999
C	5.158250000000000	8.573100000000000	13.407400000000001
C	5.066270000000000	11.698600000000001	6.773410000000000
C	5.140610000000000	13.841930000000000	9.893720000000000
C	5.118570000000000	12.111760000000000	8.157170000000001
C	5.006820000000000	10.333190000000000	6.772000000000000
C	5.029450000000000	9.912540000000000	8.154370000000000
C	5.154950000000000	13.438240000000000	8.564830000000001
C	5.079130000000000	11.677210000000001	15.207490000000000
C	5.063080000000000	12.097730000000000	13.824199999999999
C	5.126080000000000	10.311470000000000	15.202430000000000
C	5.128590000000000	9.899210000000000	13.816630000000000
O	7.430480000000000	10.814230000000000	11.074109999999999
O	9.510020000000001	9.101390000000000	13.344580000000001
O	9.147270000000001	10.814450000000001	8.886649999999999
O	9.602880000000001	13.214760000000000	10.211990000000000
O	8.102570000000000	11.667280000000000	11.979710000000001
H	5.156030000000000	9.625540000000001	16.046189999999999
H	5.067960000000000	12.384040000000001	5.928150000000000
H	4.951900000000000	9.652740000000000	5.924670000000000
H	5.125860000000000	16.073570000000000	9.633279999999999
H	5.048740000000000	16.065690000000000	12.366220000000000
H	5.063360000000000	12.358590000000000	16.055990000000001
H	4.981530000000000	5.944330000000000	9.611610000000001
H	5.109530000000000	5.940000000000000	12.343510000000000
H	5.168360000000000	14.210710000000001	7.794340000000000
H	5.038080000000000	14.196460000000000	14.194710000000001
H	4.952320000000000	7.816070000000000	7.781790000000000
H	5.204650000000000	7.800500000000000	14.175630000000000
H	9.610180000000000	12.450060000000001	9.575020000000000
H	8.985250000000001	9.810990000000000	12.924860000000001
H	10.117839999999999	9.580600000000000	13.933490000000001
H	9.163200000000000	13.940260000000000	9.735709999999999
H	8.444590000000000	10.708489999999999	9.587809999999999
H	9.780290000000001	10.096100000000000	9.060180000000001
H	8.571500000000000	12.332050000000001	11.386509999999999
N	5.112540000000000	12.995360000000000	10.991920000000000
N	5.069360000000000	9.015319999999999	10.982200000000001
N	5.094240000000000	11.010240000000000	9.000280000000000
N	5.080290000000000	11.001010000000001	12.978470000000000