

Supporting information for

Stability of surface protons in pyridine-catalyzed CO₂ reduction at p-GaP photoelectrodes

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1) Effect of solvation model and pK_a computational approach on computed pK_a s

This study was conducted in order to determine the best approach for computing pK_a s of relevant species. Getting the right trend of pK_a s for PyH^+ and HCOOH was especially important and challenging. The Solvation Model based on solute electron Density (SMD)¹ captures the correct trend (experimental $\text{HCOOH } pK_a < \text{experimental } \text{PyH}^+ pK_a$) whereas the CONductor-like Screening MOdel (COSMO)² does not. Furthermore, the direct approach, which is less computationally demanding, as explained in the main text, gives very similar results to the thermodynamic cycle approach (Figure S1). Therefore, as discussed in the main text, we used the direct approach with the SMD solvation model for all results presented in the main text. For both H_2O and H_3O^+ , the computed pK_a is far from the experimental value, independent of the solvation model and the pK_a computational approach used. As shown in Figure S4, much better agreement with the experimental value is reached when a mixed implicit-explicit solvation approach is used.

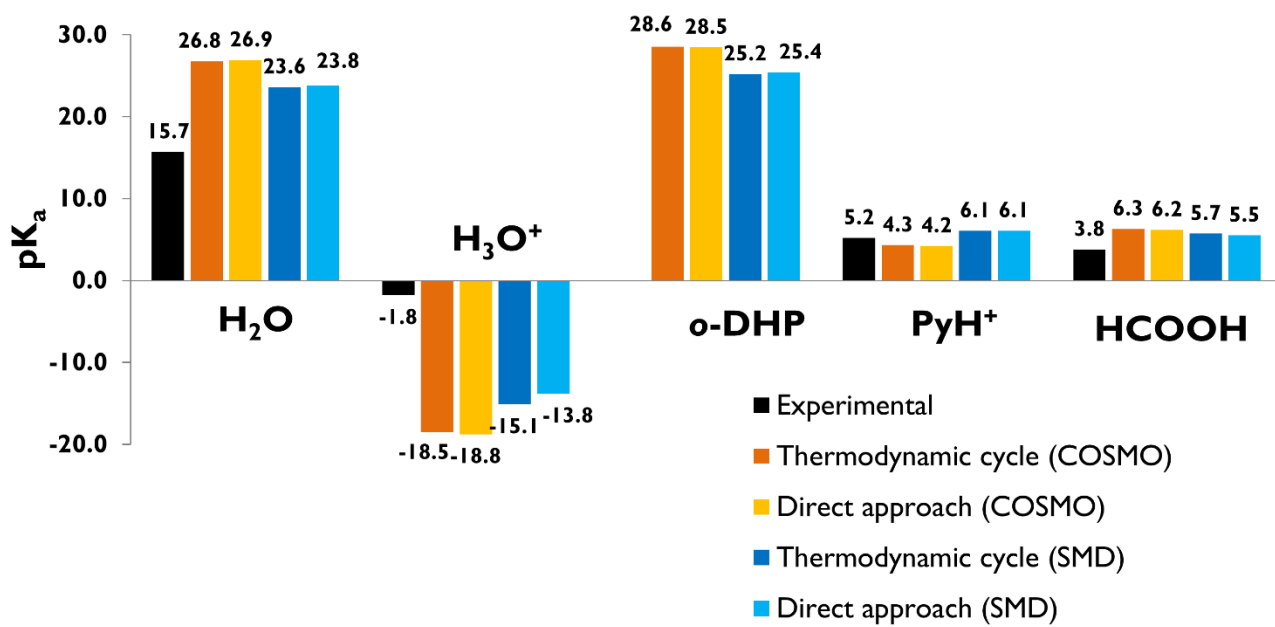


Figure S1. Effect of solvation model (COSMO vs. SMD) and pK_a computational approach (thermodynamic cycle vs. direct approach) on the computed pK_a s of relevant species in the system.

2) Cluster model

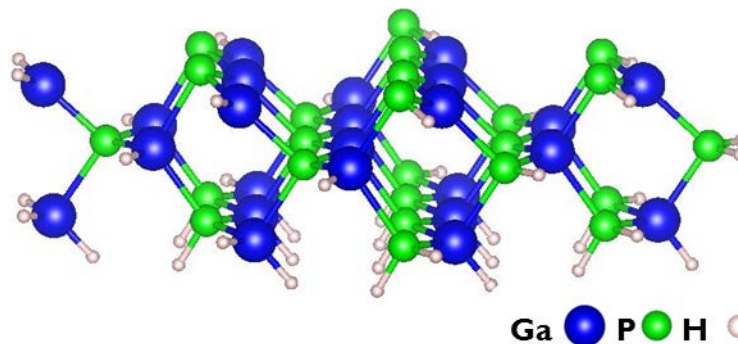


Figure S2. Cluster model used to simulate the implicitly solvated GaP(110) surface.

Details of how the cluster model was constructed are reported in the main text and in previous work.³ As a test of the model's robustness, we demonstrate that the cluster model correctly describes the electron density distribution in the GaP(110) surface when extra electrons are added to it. This is a crucial point to demonstrate, because in this study we add extra electrons to the cluster to simulate a negatively charged photocathode.

We confirmed the similarity of the relaxed geometry of the cluster model (on the right in Figure S3) and the periodic slab (on the left in Figure S3) when a hydrogen atom is adsorbed on the surface. In both cases, the electron and the proton separate, resulting in one Ga surface atom (indicated by the red circle in Figure S3) rising up to adopt an sp^3 configuration, as expected since it is hosting the extra electron, while the proton adsorbs on a surface P atom's lone pair. We see the distribution of the extra electron is the same both in the cluster model and in the periodic slab, thus confirming the validity of the former.

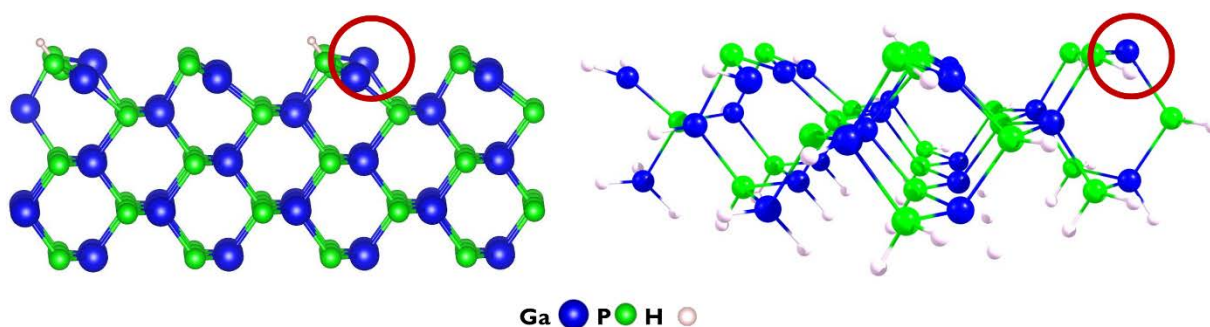


Figure S3. Periodic slab model (on the left) and cluster model (on the right) of the GaP(110) surface with an adsorbed hydrogen atom on the surface. The red circle indicates the Ga atom where the electron from the hydrogen atom localizes.

3) Effect of explicit solvation on computed pK_a s

To improve our computed pK_a s for molecules in solution, we added explicit water molecules to better account for solvation effects. For H_2O and H_3O^+ , we used known solvation structures (i.e., H_2O trimer and H_3O^+ Eigen cation with three solvating H_2O molecules). For *o*-DHP and PyH^+ , we added one water molecule to hydrogen bond to the hydrogen bound to the nitrogen atom. For $HCOOH$, we added three water molecules in total: two water molecules hydrogen-bonded to the two oxygen atoms and one water molecule hydrogen-bonded to the acidic hydrogen atom. This solvation structure was found in a previous study to give the best agreement between computed and experimental pK_a s for $HCOOH$.⁴ Except for PyH^+ , the agreement between computed and experimental values improves with a larger number of explicit solvent molecules (Figure S4).

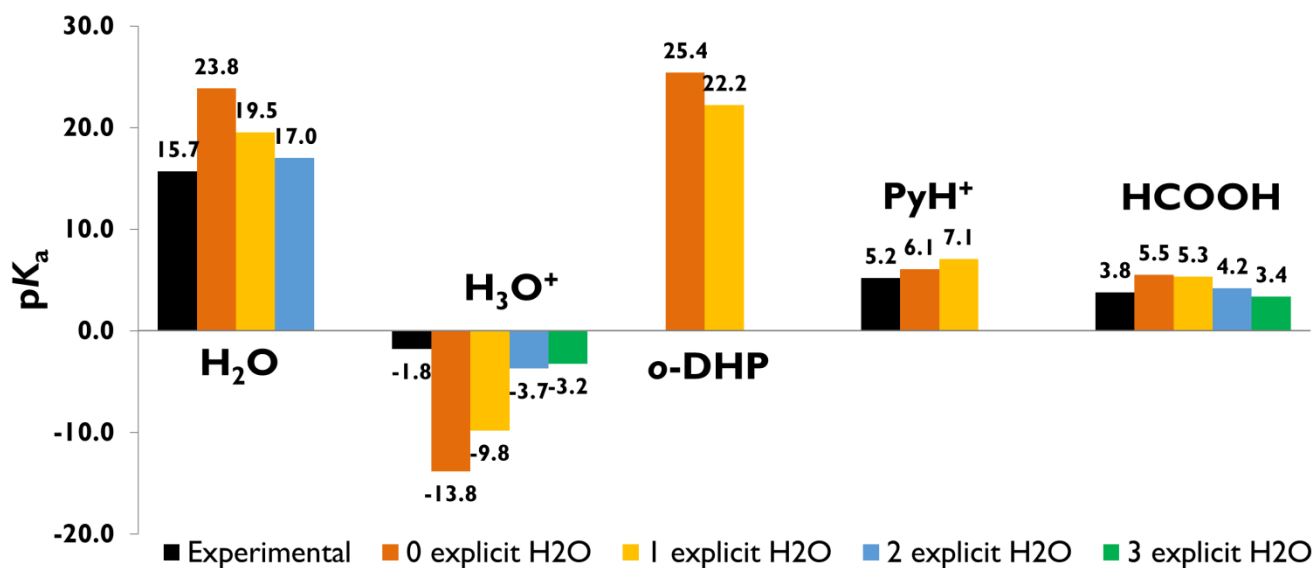


Figure S4. Effect of varying numbers of explicit solvent (water) molecules on the pK_a s of relevant species computed with the SMD solvation model and the direct approach.

4) Preferred adsorption site for protons

In this work, we modeled proton adsorption only on P surface sites. This choice is not only more intuitive but it is also supported by recent ambient pressure photoelectron spectroscopy experiments.⁵ These experiments showed that when water interacts with the GaP(110) surface, it partly dissociates leading to formation of Ga-OH and P-H species. However, these experiments were performed in the absence of an applied bias. Under this condition, Ga surface states might be occupied by the electrons deriving from the applied negative bias, thus making Ga surface atoms attractive adsorption sites for protons. To test this hypothesis, we computed the pK_a of a proton adsorbed on a Ga surface site in the case of a bare surface when different numbers of extra electrons (corresponding to different values of surface charge, as discussed in the main text) are added to the cluster model and are localized on the Ga adsorption site. These pK_a results are reported in Table S1 where they are also compared to the results for a proton adsorbed on a P surface site:

Number of extra electrons	Adsorption site	
	P	Ga
0	2.2	-31.5
1	7.4	2.7
2	13.2	28.0

Table S1. pK_a s of a proton adsorbed on the GaP(110) surface on P and Ga adsorption sites and in the presence of zero, one and two extra electrons corresponding to surface charge 0, -1, and -2, respectively.

From Table S1, it is clear that adsorption on Ga surface sites is preferred to adsorption on P surface sites only when Ga sites are hosting two extra electrons, which might occur under applied bias. However, as discussed in our recent work,⁶ the negative bias can lead to the occupation of only few Ga surface sites. Therefore, even under applied bias conditions, the P surface sites remain the major adsorption sites for protons and there is no need to consider proton adsorption on Ga sites in this work. Furthermore, even if the applied bias was to favor proton adsorption on a non-negligible number of Ga sites, the large, positive pK_a (28.0) suggests that our main conclusion does not change: adsorbed protons are very stable under experimental conditions and can potentially be reduced to hydrides and react to form the proposed active catalyst DHP.

5) Adsorption free energies

Adsorption free energies were computed using the following equation:

$$G_{\text{ads}} = G_{\text{cluster}+x} - G_{\text{cluster}} - G_x$$

where G_{ads} is the adsorption free energy of species x , $G_{\text{cluster}+x}$ is the free energy of the solvated GaP cluster-species x complex, G_{cluster} is the free energy of the solvated bare GaP cluster and G_x is the free energy of an isolated solvated x molecule. Negative values of G_{ads} indicate thermodynamically favorable adsorption while positive values indicate adsorption is unfavorable.

We computed adsorption energies using both implicit solvation (i.e., the SMD solvation model previously discussed) and a mixed implicit-explicit solvation approach. We also investigated the effect of electrode negative charge on the adsorption energies. For the mixed solvation approach, we used the SMD solvation model in the presence of a full monolayer of half-dissociated water molecules. The latter was modeled by adsorbing two $\text{H}_2\text{O}-\text{OH}^-$ complexes, three undissociated H_2O molecules and a quarter of a monolayer of protons (i.e., two adsorbed protons). This choice is explained in the next section. To simulate adsorption on the explicitly solvated surface, we removed adsorbed H_2O , OH^- and protons as needed to free the adsorption site for the species under study. Note that whenever we had to remove either an adsorbed OH^- or an adsorbed proton we removed also the adsorbed proton or the adsorbed OH^- next to it to always remove an overall neutral species. The adsorption energies obtained with both approaches (Table S2) show that the implicit solvation approach largely gives the same adsorption trend as the more accurate mixed approach (the only exception being Py which is less strongly bound with water coadsorption). We therefore decided to only use the implicit solvation scheme to study the effect of electrode negative charge on the adsorption energies. The results of this latter study are reported in Table S3. Again, roughly the same adsorption energy trend predicted for the neutral surface holds for the negatively charged surface, with formate being an exception in the case of addition of two electrons to the cluster model. This exception is readily explained given the large electrostatic repulsion between formate, a bidentate adsorbate, and the negatively charged surface.

Adsorption free energies (kcal/mol)		
Adsorbate	Implicit solvation	Implicit+explicit solvation
PyH^+	+5.5	+8.6
CO_2	+2.5	+5.2
HCOOH	-0.7	+1.7
H_2O	-2.0	-1.1
<i>o</i> -DHP	-8.2	-10.8
Py	-9.3	-6.5
HCOO^-	-13.0	-11.1
OH^-	-20.4	-21.6
$\text{H}_2\text{O}+\text{H}^+$	-25.5	-26.9

Table S2. Adsorption free energies of relevant species on the solvated GaP cluster model at 298.15 K computed using both the implicit and the mixed implicit-explicit solvation schemes. Unlike the rest of the species that adsorb molecularly intact, H_3O^+ adsorption is dissociative and produces adjacently

adsorbed $\text{H}_2\text{O}+\text{H}^+$ (hence the adsorbate entry in column 1 is shown as the latter species). Thus the H_3O^+ adsorption free energy was computed with G_x taken as the free energy of implicitly solvated H_3O^+ .

Adsorption free energies (kcal/mol)			
Adsorbate	Surface charge		
	0	-1	-2
PyH^+	+5.5	+4.7	+3.5
CO_2	+2.5	+3.3	+2.3
HCOOH	-0.7	+0.2	+0.7
H_2O	-2.0	-1.9	-2.2
o-DHP	-8.2	-8.2	-8.6
Py	-9.3	-8.4	-8.1
HCOO^-	-13.0	-9.8	-5.8
OH^-	-20.4	-19.3	-18.5
$\text{H}_2\text{O}+\text{H}^+$	-25.5	-29.4	-33.4

Table S3. Adsorption free energies of relevant species on the neutral and negatively charged implicitly solvated GaP cluster model at 298.15 K. See Table S2 for further explanation. Surface charges -1 e and -2 e were simulated by adding one and two extra electrons to the system, respectively; these correspond to approximate surface charge densities of $0.010e / \text{\AA}^2$ and $0.020e / \text{\AA}^2$, respectively, based on the surface area of the cluster model used ($96 \text{\AA}^2$).

6) Explicit solvation of the surface

As mentioned in the main text, a previous joint experimental and computational study found that in an aqueous environment, the GaP(110) surface will be fully covered by $\text{H}_2\text{O}-\text{OH}^-$ hydrogen-bonded complexes.⁵ Thus, to achieve a proper simulation of the experimental conditions in which the GaP photocathode is immersed in water, we tested the effect of adding varying numbers of $\text{H}_2\text{O}-\text{OH}^-$ hydrogen-bonded complexes on the surface of our cluster model. We considered three possible coverages for the explicitly solvated surface: only one $\text{H}_2\text{O}-\text{OH}^-$ complex ($\text{H}_2\text{O}-\text{OH}^*$), two $\text{H}_2\text{O}-\text{OH}^-$ complexes ($2 \text{H}_2\text{O}-\text{OH}^*$) and two $\text{H}_2\text{O}-\text{OH}^-$ complexes plus three undissociated water molecules ($2 \text{H}_2\text{O}-\text{OH}^*+3 \text{H}_2\text{O}^*$) on the cluster surface. As discussed in the main text, this last coverage represents a full coverage of the surface and thus best simulates experimental conditions. Both the bare surface and the surface with the different coverages mentioned above are illustrated in Figure S5.

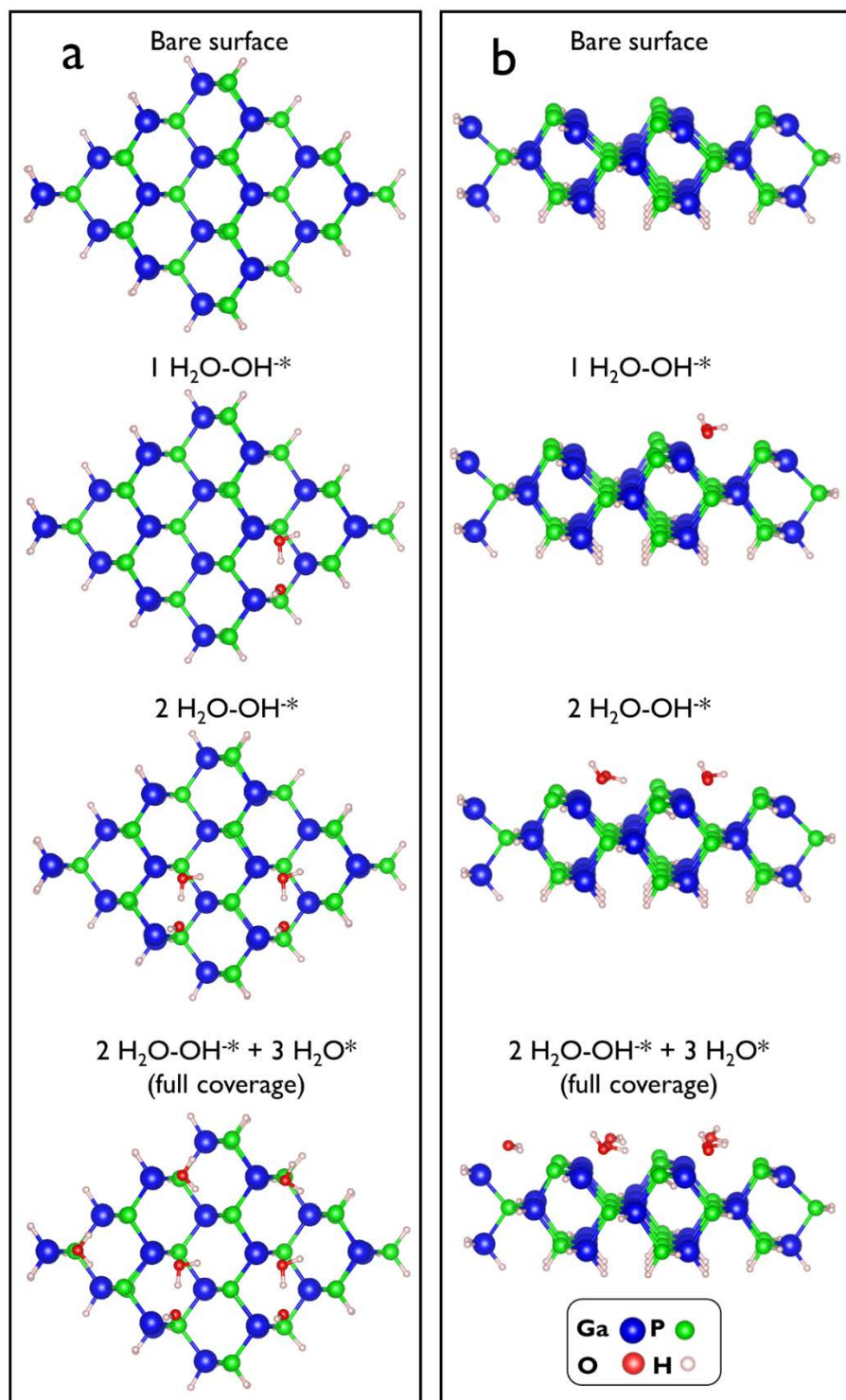


Figure S5. Top (a) and side (b) views of the GaP(110) surface cluster model with different coverages: bare surface, surface covered by only one $\text{H}_2\text{O}-\text{OH}^*$ ($\text{H}_2\text{O}-\text{OH}^*$), two $\text{H}_2\text{O}-\text{OH}^*$ complexes (2 $\text{H}_2\text{O}-\text{OH}^*$) and two $\text{H}_2\text{O}-\text{OH}^*$ complexes plus three undissociated water molecules (2 $\text{H}_2\text{O}-\text{OH}^*$ + 3 H_2O^*). * indicates species adsorbed on the surface.

For the full coverage model, we were able to add only three H_2O molecules in addition to the 2 $\text{H}_2\text{O}-\text{OH}^*$ complexes because of the geometry of the cluster model. This cluster model has eight Ga surface

sites (i.e., sites available for OH⁻ and H₂O adsorption) distributed over four Ga rows. We describe next how we decided to model the fully hydrated surface using these eight Ga adsorption sites.

The two rows at the cluster edges have one Ga site each and thus can host only one adsorbed H₂O molecule each. We did not place OH⁻ on those Ga sites because, as discussed in the previous study mentioned above,⁵ in order for OH⁻ to be stable on the GaP(110) surface, an adsorbed H₂O molecule has to be hydrogen-bonded to it. Furthermore, as seen in Figure S5, we placed an adsorbed H₂O molecule only on one of the Ga rows at the edge of the cluster, specifically the row in which the adsorbed H₂O molecule is able to hydrogen-bond to two P sites. When we tried to place an adsorbed H₂O molecule in multiple orientations on the other Ga row at the cluster edge, multiple imaginary frequencies arise associated with rotation of the molecules along the surface plane. This indicates that hydrogen-bonding between the water protons and the P sites is needed to determine the orientation of the adsorbed H₂O molecule along the surface plane and thus reach a minimum energy structure.

The two rows in the middle of the cluster each have three Ga sites. Thus, we placed one H₂O-OH⁻ complex (which occupies two neighboring Ga sites) and one H₂O molecule on each row. We chose to place an adsorbed H₂O molecule rather than an adsorbed OH⁻ because, as we just discussed, in order for OH⁻ to be stable, another hydrogen-bonded, adsorbed H₂O molecule would be required.

7) Adsorption of multiple protons on the GaP cluster

The addition of protons to the surface is schematically represented in Figure S6. The approximate coverages were calculated considering the eight possible P sites for proton adsorption on the cluster surface. Figure S6 depicts the surface P sites where protons were adsorbed on the bare surface but protons were adsorbed on the exact same P sites on the explicitly solvated surface.

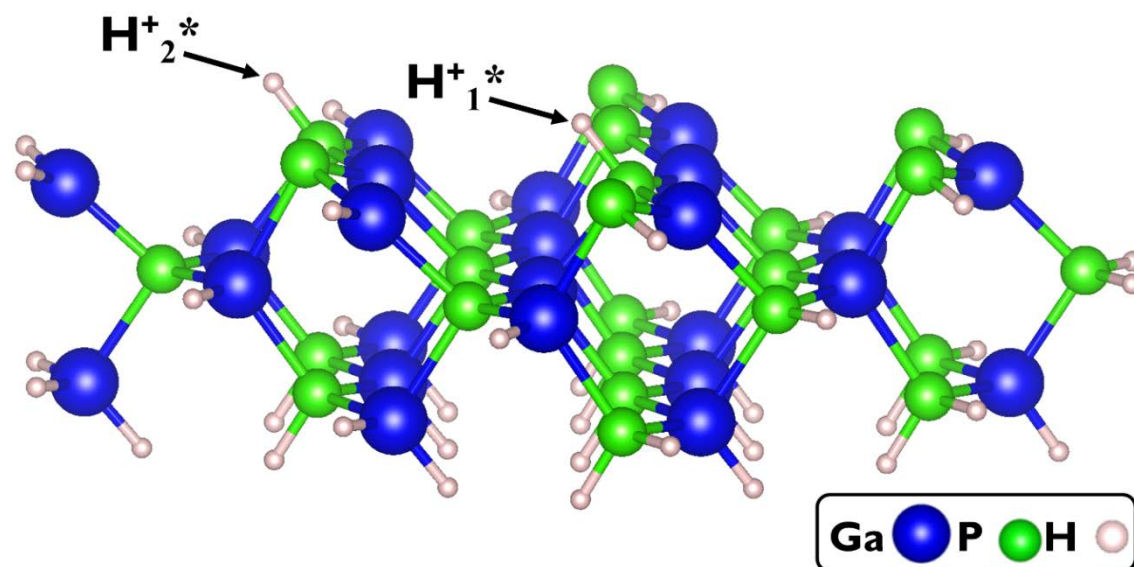


Figure S6. Proton adsorption on the GaP(110) cluster model. Proton numbering indicates the order in which protons were added to the cluster in order to simulate increasing coverages (e.g., $H^+_1^*$ is the first proton added to the cluster to simulate 0.125 ML coverage and $H^+_2^*$ is added to the cluster to simulate 0.25 ML coverage). * indicates species adsorbed on the surface.

8) References

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- (6) Lessio, M.; Senftle, T. P.; Carter, E. A. *ACS Energy Lett.* **2016**, *1*, 464–468.

9) Cartesian coordinates in Å and electronic energies in hartrees of structures discussed in the main text

pK_a calculations

1) H₃O⁺ pK_a

H₃O⁺ solvated by 3 H₂O (Eigen cation)

Energy=-306.069433591352

O	-0.62306554195262	-2.26493633967174	0.52237727755287
H	-0.31462576783932	-0.78748434941097	0.34180900809981
H	-1.19416042788085	-2.36810907366879	1.29979673133135
O	-0.09011305178466	0.21439909171759	0.30455731252337
H	0.91973068386406	0.37284286369610	0.23622795067288
H	-0.61610783335090	0.71325637103779	-0.42473673059717
O	2.43108910847206	0.62789118345064	0.24105481611554
H	2.73694741122126	0.59066523901776	1.16061390191227
H	2.59498697157282	1.54557145805992	-0.02598547371982
H	-1.15845999229003	-2.59633837182657	-0.21454359948400
H	-1.48284933028230	1.06649601651792	-2.26284363029137
O	-1.41737788697396	1.52293607000598	-1.41041358477690
H	-2.33365634277555	1.60074184107436	-1.10193997933886

H₂O solvated by 3 H₂O

Energy=-305.631208601880

O	-3.47761872623685	-1.44611240321150	-2.24907087109412
H	-2.72494572790753	-1.50496374833628	-1.60229166925314
H	-4.25914505931399	-1.34132176078850	-1.68676942309071
O	-1.42386169265243	-1.86178051355757	-0.56251998057732
H	-1.36022268654710	-2.84722253510763	-0.65241702436767
H	-0.65913164231651	-1.52387397220712	-1.04991025306400
O	-1.47435270661375	-4.56227836254103	-0.94457765703771
H	-2.16998662260930	-4.48565609152206	-1.64877364173971
H	-1.95984611500427	-4.85861406876433	-0.16126994737178
H	-2.81036490196212	-4.08897221653076	-3.65343199755426
O	-3.34496164749992	-4.08280801371964	-2.84664178903276
H	-3.47475247133623	-3.11771631371358	-2.65116574581680

2) Adsorbed HCOOH pK_a

Adsorbed HCOOH

Energy=-8455.648670966390

H	5.77741456810410	18.48719912738829	2.80454916148786
H	5.77741490056669	13.04046304069512	2.76833015123463
H	5.77741495565899	7.59241997253750	2.73413696897827
H	13.48063499756740	13.03905301681398	2.77042300908894
H	6.55859693926690	3.22350893714681	5.83627500211029
Ga	5.80437684446028	19.12664144563294	5.98498985130274
Ga	5.78312542719693	13.68156799859398	5.99399929632005
Ga	5.77130115274876	8.23883525361955	5.97306652175656
Ga	13.46116975166771	13.69430290125958	6.03710327679735
H	12.70392597515056	8.66726206249768	5.87242504665673
H	1.92580492561664	13.03905201823095	2.77042505242218
H	9.62902497734381	18.48719903103463	2.80454911471589
H	9.62902494441702	13.04046302977090	2.76833089115367
H	9.62902510079393	7.59242091106858	2.73413499763496
H	0.77682501710374	11.44172605527906	3.92960796126303
H	14.62961402441663	11.44172598042516	3.92960798596454
Ga	7.70306316926514	16.35470552373658	3.87287455513695
Ga	7.70806807653050	10.93069900104017	3.83313282743018
Ga	7.70607877747023	5.41344845951523	3.85137560103258
Ga	7.70327404433149	21.84512035825138	3.88513295567005
Ga	3.82957910716814	16.36025719841544	3.87053033556653
Ga	3.83066982439790	10.89575767258725	3.84733489350250
H	4.62962009674130	5.99564104562179	3.89357701873351
Ga	11.57810157609983	16.35993958457140	3.87038002803755
Ga	11.57577082342549	10.89376745789431	3.85047124296756
H	10.77682083152807	5.99563911992014	3.89357702126576
Ga	1.94485793971363	13.69450151006065	6.03444099446462
H	2.70251310167385	8.66726119935018	5.87242503112940
H	8.84784106960992	3.22350901370460	5.83627602617946
Ga	9.60243267299855	19.12570044956353	5.98499405922358
Ga	9.63062773031272	13.67315073395441	6.00006956597858
Ga	9.64473328704335	8.23885567153029	5.98561110544084
H	0.74840109176226	11.67346302477176	7.64098894079907
H	14.65803990442085	11.67346301739629	7.64098998266911
Ga	7.70346840704970	16.67493364544935	7.53960476155531
Ga	7.73481308130543	11.10246375043399	7.61749335690860
Ga	7.71191368211776	5.78382090057627	7.56575224085169
Ga	7.70326491998953	22.19228199274385	7.44551788296592
Ga	3.91354353491407	16.73695770048106	7.49817016519531
Ga	3.74778641658271	11.22417241071488	7.55038020678471
H	4.60139105420179	6.22734701966936	7.60533303354366
Ga	11.49517077354574	16.73473351734471	7.49382648372288
Ga	11.65144756499329	11.23150234822801	7.57233646882215
H	10.80504995275382	6.22734601176896	7.60533302256998
P	5.78563056743448	17.72212582941642	4.00511183840514
P	5.76283475032542	12.30029247494047	3.98655780407087
P	5.77110225986035	6.84730208042302	3.95441811654699

H	6.38704651996703	22.71684293849698	4.00420291845304
H	12.85194101490168	17.25642397692680	3.96807793374879
P	13.48553726446943	12.29413852424696	3.98990469732244
P	5.81459619739022	17.88730222636867	8.10880777122006
P	5.75499152876178	12.35071657951460	8.01621951249748
P	5.72901626785464	7.00860054184682	8.00385318882179
H	6.39778584590318	22.90385804513751	7.89512899101775
H	12.85064281288659	17.45114191469511	7.85597185999738
P	13.56344171549737	12.46131827003035	8.09633127018342
H	7.70321998793857	4.53002796929310	2.61196084799439
H	7.70321989212478	20.84237224802569	2.68056219749761
H	7.70322002295937	15.40326626273472	2.65531119186379
H	7.70322000963650	9.95986300962956	2.62421705894653
H	3.85160994624665	15.39798418331772	2.64793647424369
H	3.85160997588878	9.96381101213245	2.62972808950577
H	11.55483000323826	15.39798403687672	2.64793710996815
H	11.55483001044775	9.96381202834237	2.62972904616775
H	2.55450102057700	17.25642195347097	3.96807772625761
P	1.92068974255034	12.29419749745847	3.98936981205289
P	9.62122896647649	17.72168969708656	4.00486448959491
P	9.64704321629999	12.30369410396803	3.98639735151493
P	9.63829943481967	6.85044942493686	3.95766874191679
H	9.01939357274754	22.71684280678684	4.00420295605702
H	0.63926621134353	14.47657182202854	5.89317689660806
H	14.76717391589550	14.47657294148381	5.89317600595104
P	7.70356069909677	4.06870006892131	5.87200881040956
P	7.70356929573464	20.48134141450781	5.90309760399217
P	7.70673445713042	15.01942907874660	5.89339500953989
P	7.70877764365084	9.58362593571982	5.80847263747245
H	4.48385002606040	19.92840863177332	5.92900076500460
P	3.87764741022314	15.02894997679742	5.89852565368584
P	3.80551401371974	9.55779835704488	5.87066611675437
H	10.92259231362327	19.92841077322276	5.92900100353511
P	11.53037627569523	15.03096752852806	5.89309567077423
P	11.60465759751230	9.56468100673563	5.87976950178489
H	2.55579739810926	17.45114080247646	7.85597164367893
P	1.84754127779119	12.45815962374072	8.09329630236097
P	9.59383302221890	17.88528849006939	8.10818248632774
P	9.66191013686702	12.38764987764855	8.02565981803192
P	9.68759299408280	7.01280676655664	8.02134389259695
H	9.00865302146198	22.90385795452888	7.89512891243905
O	5.98694821451610	10.02470824670352	10.44967988889326
O	7.82637318006982	9.65595712401044	9.17364473932077
C	7.05080355817041	9.34996856679068	10.08940723178538
H	5.88763885410848	10.85445204892040	9.92484678430763
H	7.22245516961476	8.46235591837567	10.69871130734037

Adsorbed HCOO⁻

Energy=-8455.215947528461

H	5.77741497279906	18.48719902414440	2.80454898443683
H	5.77741497762034	13.04046301600748	2.76833001137154
H	5.77741496184554	7.59241994507081	2.73413700326203
H	13.48063512322697	13.03905292018840	2.77042303725710
H	6.55859697640160	3.22350902161804	5.83627500865987
Ga	5.80320483340333	19.12198333952955	5.98098955005406
Ga	5.76210854790502	13.73635756398188	5.91543716972568
Ga	5.74796238185367	8.25231644344476	5.98710242673982
Ga	13.45667510880727	13.69422158231082	6.04310748181963
H	12.70392600488441	8.66726199527961	5.87242501796922
H	1.92580492109687	13.03905192639330	2.77042504758040
H	9.62902500213309	18.48719900325123	2.80454902771554
H	9.62902502367547	13.04046302020180	2.76833099070944
H	9.62902501251493	7.59242094972358	2.73413502608192
H	0.77682508325005	11.44172608204426	3.92960795427854
H	14.62961387429832	11.44172611458932	3.92960796521654
Ga	7.71966385090108	16.36444820294248	3.86484394358966
Ga	7.69494531535694	10.92069328220399	3.85524447754007
Ga	7.70088612575198	5.42663714147767	3.84296091674363
Ga	7.70327802343712	21.84341514932025	3.88743127238889
Ga	3.82394842420158	16.36755302665126	3.86241834430009
Ga	3.82527326002540	10.87860120883611	3.87398756424337
H	4.62962003552913	5.99564104352067	3.89357698835627
Ga	11.57745454398587	16.34762191549543	3.88450897155526
Ga	11.56666127593523	10.89467867553280	3.85458717639235
H	10.77682096591035	5.99563903245675	3.89357698234924
Ga	1.94658777207104	13.66696845901211	6.07815869248798
H	2.70251301546082	8.66726101042535	5.87242499742226
H	8.84784103477326	3.22350896981263	5.83627599826034
Ga	9.60290459857135	19.12390889251508	5.98849244461738
Ga	9.59282734849018	13.63550798672238	6.04124677545750
Ga	9.61440884275656	8.26645600255128	5.99972138487492
H	0.74840098185936	11.67346298235272	7.64098900373615
H	14.65804007296533	11.67346297655440	7.64098998733808
Ga	7.69845085978496	16.66756588081194	7.52013162778599
Ga	7.52423995735457	11.14279115682798	7.71358325870544
Ga	7.70688339979051	5.76460024030592	7.54653352823091
Ga	7.70309541541040	22.19117863388398	7.44440489587513
Ga	3.90865721507237	16.73330107207714	7.47382726503877
Ga	3.89882721236112	11.15335200514117	7.75981892482631
H	4.60139098858724	6.22734699909890	7.60533299679593
Ga	11.49397092418693	16.72790748456995	7.49244815782712
Ga	11.61846530902361	11.22276632980616	7.58833252426221
H	10.80505001222322	6.22734599431051	7.60533300088968
P	5.78866208139490	17.71925713333061	4.00096295077957
P	5.75447267293184	12.30016404719489	3.97654190664806
P	5.76669562981246	6.85449621239711	3.95989412862939
H	6.38704602901228	22.71684297974378	4.00420298688686
H	12.85194101579011	17.25642400454531	3.96807796373408

P	13.48365164060219	12.29306748052310	3.99064193906483
P	5.81076446084360	17.88149934231401	8.10303035276995
P	5.72880265222979	12.61909434683526	7.94189006391501
P	5.74169855383707	6.97635747749209	7.99763704951806
H	6.39778619042617	22.90385801596145	7.89512894592226
H	12.85064291139677	17.45114198152146	7.85597196934493
P	13.55166822346491	12.45138422468096	8.09356248262428
H	7.70322001587768	4.53002804314250	2.61196099577570
H	7.70322005835020	20.84237210014620	2.68056210427536
H	7.70322000059596	15.40326602766296	2.65531102140745
H	7.70322000045912	9.95986296807425	2.62421699081679
H	3.85160999246980	15.39798401910378	2.64793604832170
H	3.85161000834213	9.96381101124184	2.62972802544051
H	11.55482999820687	15.39798401895645	2.64793703207358
H	11.55482999237180	9.96381203217557	2.62972901990876
H	2.55450099998615	17.25642199456896	3.96807797440673
P	1.92115988928294	12.29548060632677	3.99445689703995
P	9.62931332722734	17.72679591866751	4.00395383612644
P	9.63767759673714	12.30053741389119	3.99002333111311
P	9.63724250564824	6.85760541323120	3.96254247257691
H	9.01939388217402	22.71684293307203	4.00420297110360
H	0.63926599604984	14.47657202621691	5.89317697340454
H	14.76717389122320	14.47657294737354	5.89317599986915
P	7.70483638998461	4.06469708098710	5.85736723089281
P	7.70280206825842	20.48061145122625	5.90279849116050
P	7.71175540209565	15.03884453175942	5.85867692274390
P	7.67229360901885	9.61920779891608	5.86313016331074
H	4.48384906566273	19.92840897126186	5.92900099564355
P	3.84504202735753	15.05553154708831	5.85988635950914
P	3.79933142800099	9.58530005760221	5.90679970823057
H	10.92259297657496	19.92841099753772	5.92900099587975
P	11.50859967511495	15.00650694082925	5.90806214845385
P	11.59883382195943	9.56104580665346	5.88283627838021
H	2.55579807496818	17.45114096452899	7.85597196934933
P	1.88718614650788	12.40686221509207	8.10115268081274
P	9.58973820179531	17.87962514584333	8.10623102450609
P	9.59609594228217	12.31787655263972	8.06852810065270
P	9.67399816182402	7.00002410140426	8.01218824635236
H	9.00865282039107	22.90385794080182	7.89512896649240
O	4.59293313748887	9.91974899930390	9.29771672224848
O	6.89724920905011	9.88591067625642	9.24838507272483
C	5.74983203050408	9.62135523275446	9.73341354443577
H	5.76260709136204	9.05248850501839	10.67251623944397

3) Adsorbed H_1^+ * pK_a

Adsorbed H_1^+ *

Energy=-8266.384761079446

H	-1.94550800154733	5.15747199619123	-3.06708698189277
H	-1.92575700840103	-0.28934100580798	-3.09167999928943

H	-1.90599700372148	-5.73745700240589	-3.11424499584248
H	5.77747192353068	-0.26273194145755	-3.10184101661301
H	-1.10398998794110	-10.09690700660478	-0.00402300197650
Ga	-1.91208939558701	5.81526077809843	0.11044684821616
Ga	-1.92049034463655	0.42082917465628	0.00526128120237
Ga	-1.92265863450657	-5.11370443728225	0.13497706186682
Ga	5.76801810418593	0.39535286874756	0.16602698154495
H	5.02159799283106	-4.63072599171254	0.01072799173999
H	-5.77735803164432	-0.30475602540085	-3.08345299199295
H	1.90610201831979	5.17148000720361	-3.07321599044268
H	1.92585298625281	-0.27533299976883	-3.09780701215042
H	1.94561196435555	-5.72344796305486	-3.12037402149342
H	-6.91868397020145	-1.90378497255149	-1.91903300882891
H	6.93410409139262	-1.85340607661928	-1.94107598750071
Ga	-0.00142779334344	3.05404742365403	-2.01476504336935
Ga	0.03616094446961	-2.37900435179349	-2.04151619514195
Ga	0.03048149329836	-7.91716572445972	-1.99145679064373
Ga	-0.03012210089336	8.52883837873191	-2.00168790283149
Ga	-3.88448095742318	3.03971970670627	-2.00815038191406
Ga	-3.88606664402876	-2.43539936922261	-2.01764206558282
H	-3.04613999883835	-7.33593599855971	-1.94956900153818
Ga	3.86607545518337	3.06060414196752	-2.01526347813709
Ga	3.90233574385625	-2.41212228663801	-2.02078005228816
H	3.10106004036361	-7.31358103926739	-1.95935098404419
Ga	-5.76110436350378	0.35394212898790	0.16792825846652
H	-4.97981399860951	-4.66709999593466	0.02664299952194
H	1.18525398605824	-10.08857999123397	-0.00766599922120
Ga	1.88201118181417	5.82437431416628	0.11169522914179
Ga	1.94986000562085	0.38730180288363	0.11492087207422
Ga	1.99324643964907	-5.10068611871264	0.11261905184356
H	-6.94204600232841	-1.66423100018164	1.79189899942527
H	6.96759297591408	-1.61364399287507	1.76976600041961
Ga	-0.00285394644390	3.37714019136615	1.67368698574074
Ga	0.19719312262989	-2.17606623168107	1.64151913393892
Ga	0.03886987898344	-7.53999304626164	1.72530634385069
Ga	-0.02575558474787	8.88319603756066	1.56425896353639
Ga	-3.79036695761067	3.43175781549478	1.63994118586581
Ga	-4.09161737493082	-2.19010157660604	1.73256924519696
H	-3.06930600271415	-7.09640899902062	1.76173699987763
Ga	3.78603356658188	3.44455079391900	1.62408419254545
Ga	3.99988587134113	-2.08178315215613	1.71082698345088
H	3.13435300015528	-7.07384899919790	1.75186599990889
P	-1.93037915607499	4.39879644905326	-1.86349498793697
P	-1.93603394486989	-1.04503545800028	-1.89222922068857
P	-1.90705110950158	-6.48161835120111	-1.89476649273969
H	-1.34935100977579	9.39189399195919	-1.87743100575791
H	5.13534500834086	3.95490901665242	-1.91218799948773
P	5.79343246778470	-1.00037028945413	-1.88029730731416
P	-1.89272188645857	4.57791456537176	2.24339049389532

P	-1.93910077430898	-1.15271120848360	1.89226897049077
P	-1.94587745169628	-6.31310171267392	2.17034511095993
H	-1.33309892954437	9.58725300776903	2.01307798068193
H	5.13952506628732	4.15792202180659	1.97529201678154
P	5.88183074910574	-0.82283260167773	2.23407436442492
H	0.03075000053209	-8.79310600771796	-3.23294800033382
H	-0.02846596566300	7.51938504718136	-3.19916495281181
H	-0.00872399986440	2.08022498219089	-3.21280702536186
H	0.01102300281994	-3.36324499327585	-3.23228200084888
H	-3.86032698870415	2.06091898285738	-3.21404100427204
H	-3.84059299358619	-3.37329199972280	-3.22065100551868
H	3.84289299051498	2.08893498182315	-3.22629800897193
H	3.86262700857858	-3.34527700430281	-3.23290699039557
H	-5.16209401878881	3.91745701489396	-1.89580299319936
P	-5.78432040029554	-1.04389282109784	-1.86401169231899
P	1.90840910638605	4.41632588400474	-1.86896852587890
P	1.96266581679374	-1.00634579293393	-1.87725499387822
P	1.95700937490859	-6.47088009133879	-1.90419125338803
H	1.28299796929451	9.40146697840606	-1.88162001686023
H	-7.06415598335748	1.13475100234148	0.03827800185228
H	7.06375199805456	1.18613299801730	0.01579699959799
P	0.03830672578248	-9.24982862686674	0.03142086413985
P	-0.01932269241125	7.17077816814937	0.02244441081997
P	0.01488569246121	1.71545778114564	0.02549845161659
P	0.03099201574357	-3.76436765928350	-0.05476798865206
H	-3.23934400935128	6.60064702100340	0.05634699126596
P	-3.84205150856941	1.71140327078469	0.04314197210042
P	-3.88339623644612	-3.77505306199093	0.01196894800147
H	3.19939993877180	6.62406496325159	0.04610199496888
P	3.83856701570366	1.73876208350640	0.02256411609154
P	3.92244931244734	-3.73505900359430	0.01315636385299
H	-5.15532101239169	4.12048000853057	1.99167300659056
P	-5.88215403903772	-0.84337900453924	2.26581436342335
P	1.88218072339856	4.58659860502988	2.23565772896500
P	2.01860249952425	-0.88499310676819	2.19325246373678
P	2.00906427301955	-6.29264948237378	2.15728220890923
H	1.27776794190464	9.59674898647021	2.00892399255309
H	-1.93101367340666	-0.30297334319837	3.01146356393572

Bare cluster

Energy=-8265.939624295232

H	5.77741509490020	18.48719921390018	2.80454894007182
H	5.77741498812246	13.04046336138362	2.76833019898295
H	5.77741495274477	7.59242012354116	2.73413661500088
H	13.48063513531898	13.03905255847472	2.77042347175199
H	6.55859726825646	3.22350853114381	5.83627544310968
Ga	5.80457098120444	19.12788470962892	5.98592318984216
Ga	5.77150462998150	13.69013859011857	5.99118677441102
Ga	5.75153402418108	8.22784198667444	5.97524904320101

Ga	13.46363524493549	13.69308293846141	6.03927939661856
H	12.70392629799416	8.66726174650324	5.87242507905695
H	1.92580489365155	13.03905173593185	2.77042468113574
H	9.62902518205179	18.48719933883104	2.80454881888631
H	9.62902504193717	13.04046304845870	2.76833075761500
H	9.62902483101408	7.59242106254641	2.73413534925140
H	0.77682480951740	11.44172611594141	3.92960749139789
H	14.62961382847455	11.44172607185685	3.92960798367365
Ga	7.70323974389301	16.35829317051818	3.86978734616578
Ga	7.70318828102244	10.93751579108018	3.82780494943320
Ga	7.70297963074835	5.41009526122332	3.85192394594860
Ga	7.70316666434108	21.84533296730331	3.88519575213824
Ga	3.82903075161669	16.36291688360483	3.86785799828400
Ga	3.82564820796910	10.89719284624022	3.84529409059226
H	4.62962021541021	5.99564051145907	3.89357732404267
Ga	11.57745355454096	16.36278662307704	3.86799290424486
Ga	11.58058370177451	10.89703946082913	3.84547445361306
H	10.77682057449097	5.99563916737267	3.89357708588979
Ga	1.94322339219128	13.69366922113659	6.03929740809750
H	2.70251339677096	8.66726130653609	5.87242543204201
H	8.84784146138954	3.22350887244045	5.83627573350024
Ga	9.60180510595994	19.12790570508500	5.98582319122899
Ga	9.63498364334801	13.69037366286882	5.99116255095286
Ga	9.65470635872160	8.22790751355718	5.97527755833616
H	0.74840068280233	11.67346250384625	7.64098897652823
H	14.65803971864639	11.67346263053859	7.64098961657253
Ga	7.70323705742172	16.67536815061378	7.53820980096770
Ga	7.70309687030807	11.21263232239477	7.48452036841962
Ga	7.70311307239963	5.77859013200736	7.56784811369931
Ga	7.70323959016135	22.19162512492932	7.44740796471265
Ga	3.91361826143862	16.74020382803608	7.49883150762794
Ga	3.75281104560263	11.22267521664049	7.56156380272521
H	4.60139088823942	6.22734726967417	7.60533347859793
Ga	11.49304813651693	16.74001299235609	7.49850617837789
Ga	11.65351480339474	11.22273916338885	7.56171371607770
H	10.80504970133127	6.22734636305598	7.60533301845793
P	5.78544006062019	17.72341425833362	4.00521132934048
P	5.75822945199364	12.30447704636218	3.98691637717995
P	5.77035600561935	6.84625285273073	3.95308512053776
H	6.38704559480350	22.71684350250197	4.00420322304975
H	12.85194068188020	17.25642362749087	3.96807758575361
P	13.48784023607545	12.29611788751149	3.99009931375138
P	5.81550407153651	17.88893015616866	8.10910370377089
P	5.74771928082109	12.37771799324554	8.02789079427494
P	5.72552712734293	7.00979287307090	8.00967472822783
H	6.39778587851562	22.90385778605612	7.89512878182251
H	12.85064297611968	17.45114198195308	7.85597214783571
P	13.55965885057806	12.45772231523258	8.09526974814976
H	7.70321980671840	4.53002828598865	2.61196079683769

H	7.70321993869830	20.84237163311758	2.68056178595769
H	7.70322004385983	15.40326646124848	2.65531097724938
H	7.70321992713148	9.95986313438714	2.62421713586267
H	3.85161008795817	15.39798395194255	2.64793619634648
H	3.85160995522272	9.96381134705805	2.62972785850249
H	11.55483001067409	15.39798433754153	2.64793738741381
H	11.55482989609996	9.96381195559084	2.62972867855443
H	2.55450145105245	17.25642182700429	3.96807764536304
P	1.91844994290519	12.29625433066640	3.99016599210626
P	9.62103459919796	17.72338292198955	4.00521063092944
P	9.64813203604329	12.30449141418994	3.98694671177024
P	9.63605609299085	6.84608153617373	3.95291228358510
H	9.01939449631178	22.71684278408522	4.00420265738153
H	0.63926646308960	14.47657185796088	5.89317720809514
H	14.76717408901653	14.47657318399810	5.89317633906440
P	7.70320374455922	4.06664499122506	5.87240382248287
P	7.70321435527970	20.48312743637683	5.90278912390322
P	7.70318419620195	15.02292193796637	5.88867772670538
P	7.70311655201459	9.56137349716060	5.81314318783985
H	4.48384901899292	19.92840925572431	5.92900073053647
P	3.87051900932263	15.03672527006105	5.89573640529920
P	3.80187268123003	9.56224140698820	5.87066864596906
H	10.92259262817315	19.92841059161561	5.92900143126895
P	11.53630281796108	15.03642983457313	5.89582638533716
P	11.60447583149745	9.56214650676216	5.87064543302017
H	2.55579668630099	17.45114108785556	7.85597167251685
P	1.84684774285384	12.45780174839783	8.09515986238563
P	9.59107941027158	17.88866429935808	8.10890769039205
P	9.65855111092305	12.37757237633334	8.02771476008071
P	9.68076526366349	7.00969126068583	8.00962574131642
H	9.00865301829845	22.90385828029916	7.89512908072084

4) HCOOH pK_a

HCOOH solvated by 3 H₂O

Energy=-418.895386403010

O	-0.19406117091134	1.12199739028942	0.42741931133450
O	-0.12160593408815	-0.54266158707836	-1.09949873757684
C	-0.00800427103207	-0.13138783392780	0.05231638854292
H	-0.45108470724247	1.67547106342980	-0.38891978425924
H	0.26872055803305	-0.77841357527111	0.89328101458450
O	-0.82725430552878	2.19043300659558	-1.84028385589280
H	-0.83540383382458	1.31524422059319	-2.26474714232910
H	-0.06008587723103	2.63756243564835	-2.22806284865008
O	0.52952550812601	-3.23291348254796	-0.56092670509739
H	1.49261820615116	-3.23784571278564	-0.64430308851916
H	0.27442463568096	-2.36346763810643	-0.92269970344693
O	0.72084726857287	0.69647168235562	3.15568799093574
H	-0.09440520811214	0.38467327230810	3.57222693114544
H	0.40954313140650	1.11072175849723	2.33496922922845

HCOO⁻ solvated by 3 H₂O

Energy=-418.429712508534

O	-0.00388057734058	1.15920420334305	0.36689214189057
O	0.13274586753076	-0.53748977441852	-1.12071615323230
C	0.26552338653466	-0.03048267618679	0.03034659833399
H	0.65849695594558	-0.69563836561966	0.82726636541903
O	-1.44739206409090	1.61606820465444	-2.02335725606845
H	-1.00597588933788	0.75223079148905	-2.12709593996446
H	-1.09102087832481	1.83490369030723	-1.14146156587756
O	0.58713131955917	-3.15851732198505	-0.49315653817780
H	1.51193857536987	-3.15052832623524	-0.21136265730090
H	0.44057953419966	-2.24293255432778	-0.82718248415552
O	0.75840683302590	0.88135974191495	2.99384755967419
H	0.00764866376842	0.37499722290096	3.33297881757470
H	0.47060427316014	1.12338216416336	2.08366511188451

5) PyH⁺ pK_a

PyH⁺ solvated by 1 H₂O

Energy=-325.021009755531

C	-1.33664618437306	0.42009147553094	-1.27414857066976
C	0.03818167526169	0.42495134320998	-1.10014428555735
C	-0.18368205687126	-0.43188837824943	1.08994321846985
C	-1.56415846994082	-0.45832745637997	0.96901514933443
C	-2.14656849381109	-0.02734859035903	-0.22703619627313
H	-3.22480256399219	-0.03974125052118	-0.34465437599542
H	-2.16709375706197	-0.80893407655230	1.79674035381049
H	0.34923249188649	-0.74660822720074	1.97747615106714
H	0.73670761841647	0.75571757310058	-1.85692486372097
H	-1.76118625952078	0.76295133471031	-2.20906493176662
N	0.57103631508238	0.00304546885267	0.06306019031112
H	1.61568723095764	0.02090972025683	0.17976369406986
O	3.26005194546520	0.03135538108414	0.38021205500349
H	3.62998595452602	-0.63681406031885	-0.21550558796580
H	3.59846855397529	0.87104674283606	0.03508799988266

Py solvated by 1 H₂O

Energy=-324.550774509111

C	-2.84664554067819	0.25209081488971	-3.19773752931038
C	-1.52327753162729	0.36195364480419	-2.76902373074230
C	-2.07904003425176	-0.26975536638702	-0.62830356950871
C	-3.42546123888959	-0.40632460917404	-0.96192923888077
C	-3.81814916096233	-0.13964738937540	-2.27536136288019
H	-4.85674428443458	-0.23760203568161	-2.57625944611823
H	-4.14226232635376	-0.71696249373990	-0.20980518693645
H	-1.72820802094439	-0.47569472222625	0.37919571182402
H	-0.74498924614558	0.66639810220497	-3.46339550128945
H	-3.10625544477891	0.47297152169554	-4.22748160816840
N	-1.13258376920018	0.10853458720049	-1.50690848166206

O	0.89881582887500	-0.05395580070554	0.49942401759600
H	0.37241911476498	0.05417316273786	-0.32222143483878
H	0.73612185935630	0.77117649512702	0.97654182206424

6) Adsorbed H₂O pK_a

Adsorbed H₂O

Energy=-8342.36805693211

H	5.77741513363586	18.48719921594847	2.80454894287731
H	5.77741500160075	13.04046333415740	2.76833019866427
H	5.77741494860681	7.59242012258956	2.73413662144934
H	13.48063509420468	13.03905258264744	2.77042346877850
H	6.55859728200130	3.22350852235422	5.83627544144321
Ga	5.80357587537743	19.10552873054439	6.01489315049379
Ga	5.78784666129124	13.70550897188475	5.96285121905592
Ga	5.75123666265675	8.23106248401148	5.97758885655117
Ga	13.46111549910565	13.69660415213995	6.03449958204208
H	12.70392631188991	8.66726172691831	5.87242507180815
H	1.92580492252957	13.03905173550538	2.77042468716288
H	9.62902516066451	18.48719935659419	2.80454885006676
H	9.62902502758732	13.04046303066178	2.76833076091582
H	9.62902483145870	7.59242106229864	2.73413535661410
H	0.77682478414692	11.44172610451460	3.92960749597112
H	14.62961387342825	11.44172603173276	3.92960798758786
Ga	7.70327719325978	16.36398201319894	3.86735478047831
Ga	7.70310586413568	10.93808119402812	3.82631141876059
Ga	7.70294379396975	5.41071718086965	3.85230144457964
Ga	7.70314308073295	21.83696525336964	3.89549486961483
Ga	3.83298670953489	16.36574555319072	3.86852877686298
Ga	3.82406567623179	10.89629421012583	3.84575643991396
H	4.62962022373075	5.99564051759726	3.89357732652188
Ga	11.57351666947644	16.36562061148859	3.86865022814353
Ga	11.58211671767924	10.89607118280909	3.84598097940065
H	10.77682057572588	5.99563917169979	3.89357708688225
Ga	1.94568973948354	13.69711602185945	6.03450921486946
H	2.70251338358609	8.66726128644712	5.87242543031725
H	8.84784143986981	3.22350888054592	5.83627573305226
Ga	9.60287427979896	19.10537883713660	6.01492059951425
Ga	9.61859736010861	13.70564734340824	5.96296791718280
Ga	9.65500020381309	8.23114785960946	5.97766039112887
H	0.74840068980194	11.67346251413026	7.64098898134252
H	14.65803971368107	11.67346263330949	7.64098962160456
Ga	7.70326848222271	16.53191678568457	7.70058412038220
Ga	7.70312400098613	11.22166071286037	7.48335169357286
Ga	7.70312835052509	5.77939697508529	7.56807417601093
Ga	7.70324041338837	22.18566195410195	7.44841081800032
Ga	3.91474435772481	16.73363895115101	7.51062835450687
Ga	3.74641828655187	11.23642966734954	7.56686488588238
H	4.60139089179482	6.22734727570625	7.60533347831873
Ga	11.49187550149475	16.73332605925911	7.51036700675279

Ga	11.65997755925412	11.23658743893810	7.56715357090460
H	10.80504969687065	6.22734636990971	7.60533301828196
P	5.78615894301216	17.72620818736516	4.00760355354667
P	5.75721717313329	12.30078418911257	3.98308813415384
P	5.77008047110723	6.84796470060890	3.95422184218158
H	6.38704558413799	22.71684349923438	4.00420322336414
H	12.85194066509605	17.25642360151933	3.96807756666155
P	13.48776103644090	12.29599217589597	3.99000303660067
P	5.82280414854316	17.86054634805440	8.11920174690357
P	5.75146871981130	12.39477762408679	8.01037475244934
P	5.72569925483606	7.01025984043563	8.01043686814945
H	6.39778575183191	22.90385777549870	7.89512881113338
H	12.85064295498349	17.45114197177477	7.85597215643434
P	13.56602253834374	12.46688861970705	8.09728171041664
H	7.70321980323758	4.53002828282421	2.61196079262470
H	7.70321991677109	20.84237160206866	2.68056175733227
H	7.70322002207680	15.40326644398407	2.65531102089659
H	7.70321992830614	9.95986313921219	2.62421710356045
H	3.85161005381393	15.39798398110120	2.64793618689515
H	3.85160995302601	9.96381134712836	2.62972783389617
H	11.55483003356084	15.39798434360084	2.64793738576305
H	11.55482990047901	9.96381195007054	2.62972866587198
H	2.55450149614547	17.25642178253627	3.96807764472085
P	1.91853645189784	12.29620430567871	3.99001535925338
P	9.62035059557854	17.72619463487340	4.00760154256636
P	9.64909096123978	12.30075270392458	3.98313009470824
P	9.63626911552458	6.84779419490197	3.95407140955402
H	9.01939453740764	22.71684279464930	4.00420265990521
H	0.63926641179605	14.47657187110901	5.89317721254330
H	14.76717410187091	14.47657319084515	5.89317634477232
P	7.70320556163198	4.06739386314769	5.87263661112331
P	7.70329314878587	20.46896952622009	5.91314048764080
P	7.70319590433596	15.05120721548587	5.87006501592525
P	7.70313339722767	9.56732604976026	5.81702151017861
H	4.48384897945547	19.92840931076307	5.92900070216703
P	3.87260091481549	15.03560121283256	5.89635633570200
P	3.80122896716111	9.56771416361722	5.87627352636601
H	10.92259268603924	19.92841066246426	5.92900140720866
P	11.53412937861456	15.03522470002832	5.89639340803267
P	11.60514883171542	9.56764910113921	5.87640282594704
H	2.55579670460470	17.45114106784693	7.85597167606530
P	1.84049194287110	12.46679752554291	8.09711832259921
P	9.58379973712955	17.86026482062017	8.11902155913817
P	9.65476041349754	12.39465856729434	8.01057386400222
P	9.68065297811926	7.01013121169101	8.01040018635154
H	9.00865314581833	22.90385831335644	7.89512909893005
O	7.70265045295666	15.00239394568193	9.26614779427137
H	8.47760233236447	14.40564436473966	9.21097789505541
H	6.93093569380238	14.40181745565679	9.20670401673499

Adsorbed OH⁻

Energy=-8341.89616776371

H	5.77741516647758	18.48719923276371	2.80454893759060
H	5.77741503114899	13.04046332918942	2.76833020527215
H	5.77741494662350	7.59242010875636	2.73413663038969
H	13.48063502610929	13.03905263351855	2.77042344793013
H	6.55859724636511	3.22350853118722	5.83627543804322
Ga	5.80929400811438	19.10473222853437	6.01276396489934
Ga	5.81340369538439	13.73756069792599	5.99212741225470
Ga	5.75250003341683	8.23343166545036	5.97613767268026
Ga	13.45132197748828	13.70701163509325	6.03697100968079
H	12.70392630435922	8.66726171264251	5.87242504608843
H	1.92580500216959	13.03905178012138	2.77042464588490
H	9.62902513776316	18.48719937076048	2.80454884676254
H	9.62902500479336	13.04046304911260	2.76833078142121
H	9.62902488611930	7.59242099800360	2.73413538995983
H	0.77682474083524	11.44172605638888	3.92960755284354
H	14.62961391955039	11.44172598362902	3.92960800990594
Ga	7.70226474983143	16.34642294390736	3.89717843385793
Ga	7.70141089932391	10.94693491142149	3.82345123950300
Ga	7.70354541991578	5.41228039348101	3.85173395019691
Ga	7.70315670087215	21.83753181385095	3.89509768794504
Ga	3.83829677601409	16.36355749116745	3.87804889081094
Ga	3.83627014865066	10.90445009122243	3.84466027056608
H	4.62962023639410	5.99564052609586	3.89357732501089
Ga	11.56854655123037	16.36301952307502	3.87866281558336
Ga	11.57066573278067	10.90241536009531	3.84621555442356
H	10.77682050470225	5.99563923504959	3.89357706847900
Ga	1.95457400642808	13.70632687938029	6.03883570287727
H	2.70251335565342	8.66726124751465	5.87242542866869
H	8.84784147864685	3.22350886584397	5.83627573723094
Ga	9.59708904079744	19.10524836040217	6.01075778730405
Ga	9.59290872415666	13.73629473148248	5.98799573664008
Ga	9.65488870240663	8.23468266953329	5.97687521277660
H	0.74840074604348	11.67346254435550	7.64098899600029
H	14.65803966747264	11.67346265151739	7.64098963420765
Ga	7.70416628899335	16.47378886038398	7.93357876232036
Ga	7.70336453641778	11.21799489699504	7.47374548570870
Ga	7.70325120759295	5.78084001085668	7.56664412120243
Ga	7.70328826611839	22.18594877318644	7.43933112603983
Ga	3.93799717313159	16.76342706953908	7.52489809892768
Ga	3.76362765120110	11.23702625352021	7.55250905468809
H	4.60139090443451	6.22734728361001	7.60533347756871
Ga	11.46800273178171	16.76465055922603	7.52496388926708
Ga	11.64347304368301	11.24032300778417	7.55474604995449
H	10.80504970507823	6.22734636934299	7.60533301600330
P	5.78973333245901	17.72626695407984	4.00747511281195
P	5.76164929543592	12.31852833105455	3.99629791564182

P	5.77043459012960	6.84734729961628	3.95451348891707
H	6.38704562652749	22.71684344414349	4.00420320380972
H	12.85194071213030	17.25642366657566	3.96807764322518
P	13.48551635979174	12.29670930715476	3.99151099282816
P	5.83102696362382	17.91405792974808	8.10509975326956
P	5.75724476118774	12.38750045954038	8.01970181283960
P	5.72586153176909	7.01026388702678	8.00898085901457
H	6.39778593816860	22.90385778864098	7.89512876313143
H	12.85064295740524	17.45114196243546	7.85597216363165
P	13.55903925784878	12.46042334693693	8.09163728350098
H	7.70321980412826	4.53002829233155	2.61196077136542
H	7.70321997294892	20.84237172874586	2.68056189155306
H	7.70322001876428	15.40326642911085	2.65531105023440
H	7.70321992336321	9.95986315358429	2.62421713034316
H	3.85161004609104	15.39798397952925	2.64793619000158
H	3.85160993887076	9.96381132884427	2.62972778911972
H	11.55482999965046	15.39798425248293	2.64793729753882
H	11.55482992034915	9.96381188832449	2.62972864273628
H	2.55450150976912	17.25642176909377	3.96807765387805
P	1.92061724113381	12.29709945391765	3.99187427492868
P	9.61636563413191	17.72554331112533	4.00701667785121
P	9.64417965031723	12.31665500707097	3.99512131253603
P	9.63641641505131	6.84782288732234	3.95490959682509
H	9.01939441871253	22.71684271959823	4.00420262538158
H	0.63926626203706	14.47657190645421	5.89317720986659
H	14.76717420281356	14.47657324214821	5.89317634832181
P	7.70318006072995	4.06802927548316	5.87180125426949
P	7.70304774279347	20.47775160113835	5.89982262852880
P	7.70303114774670	15.11296730517573	5.94809801927871
P	7.70323591346267	9.56284787856402	5.80812466839561
H	4.48384888695380	19.92840936654758	5.92900069789922
P	3.87937402223054	15.04699633320869	5.91396996862469
P	3.80210850983090	9.56518442312161	5.86961566109457
H	10.92259271558486	19.92841067701213	5.92900140969403
P	11.52640720528014	15.04702595449980	5.91493457139942
P	11.60535591438161	9.56616838711287	5.87176293965710
H	2.55579677449607	17.45114104660347	7.85597165786281
P	1.84898883009797	12.45895739679294	8.09145438660805
P	9.57559708674673	17.91681983500926	8.10458154074329
P	9.64876395618002	12.38931314158896	8.01796751403661
P	9.68050425319461	7.01020690808661	8.00903204656832
H	9.00865297247757	22.90385825524587	7.89512907142640
O	7.70635567128669	15.30107632309140	9.43806442156114
H	7.71241850767177	14.37786600603439	9.14387593972787

7) Adsorbed *o*-DHP pK_a

Adsorbed *o*-DHP

Energy=-8515.29655222234

H	5.77741510482199	18.48719913429732	2.80454891492926
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H	5.77741498963069	13.04046330934358	2.76833018649507
H	5.77741487876274	7.59242005213041	2.73413667600804
H	13.48063513974616	13.03905257217330	2.77042345282988
H	6.55859720229205	3.22350856738579	5.83627543634115
Ga	5.80329393493846	19.12348834061107	5.98482225950254
Ga	5.78363882594719	13.66965938671592	5.98675830945942
Ga	5.77370264307130	8.24872255660391	5.96077281698130
Ga	13.45692666344762	13.70139918029987	6.03349048927113
H	12.70392635996757	8.66726176414295	5.87242506332829
H	1.92580490553160	13.03905176595875	2.77042463091440
H	9.62902515376703	18.48719928814478	2.80454879574622
H	9.62902502277429	13.04046300689125	2.76833076925418
H	9.62902495747420	7.59242095062585	2.73413538849448
H	0.77682480772918	11.44172608375783	3.92960751881169
H	14.62961384130395	11.44172605435371	3.92960799106069
Ga	7.70425977506234	16.35474603980913	3.87287127133234
Ga	7.70240555428167	10.92459102986191	3.84747751734382
Ga	7.70400887723122	5.41988442659701	3.84362557016576
Ga	7.70312977012195	21.84405341378859	3.88666035563646
Ga	3.82697485443604	16.35844969569562	3.87210019676618
Ga	3.83196768617943	10.89334437056922	3.85264552427242
H	4.62962030358752	5.99564059195171	3.89357730511412
Ga	11.57738306674644	16.36025834762122	3.87100983579175
Ga	11.57593556646557	10.89525878346062	3.84949493323423
H	10.77682042157203	5.99563929323788	3.89357704680571
Ga	1.94468935952409	13.69271342035601	6.03847041460712
H	2.70251338367701	8.66726127165434	5.87242542855138
H	8.84784154780801	3.22350882754815	5.83627573936809
Ga	9.60234079146910	19.12496763055624	5.98516926665955
Ga	9.62360734139164	13.66545603769530	5.99074010816763
Ga	9.63002656191530	8.25274638690430	5.96890354888727
H	0.74235903978640	11.64697401004234	7.64093316715797
H	14.65193822945341	11.67486488273705	7.61113872201739
Ga	7.70356493426338	16.66783538915783	7.53080823364334
Ga	7.68600427890599	11.11572656173512	7.73039895026194
Ga	7.70986043422812	5.75765154705216	7.54077693430928
Ga	7.70320363241189	22.19027813345270	7.44701611399442
Ga	3.91006769631474	16.73079306715325	7.48991047225469
Ga	3.77151293861745	11.24940473662355	7.57113433206118
H	4.60139081272906	6.22734722311389	7.60533346756464
Ga	11.49467332205655	16.73405689577115	7.49133408624477
Ga	11.64138325058502	11.24568639843092	7.55558119843188
H	10.80504967580744	6.22734640728929	7.60533304385766
P	5.78500189376280	17.72081483726268	4.00378887058547
P	5.76163685350469	12.30025787524719	3.98232163777955
P	5.77006059204798	6.84960051249092	3.95281364159593
H	6.38704568607183	22.71684347101522	4.00420320251013
H	12.85194059996167	17.25642353063251	3.96807755460211
P	13.48615087863218	12.29501876396886	3.99006291115411

P	5.81353245924162	17.87953024633940	8.10551303813417
P	5.74277565203674	12.42506723417663	8.01740795941802
P	5.74445317183041	6.99130631312762	7.97605821806230
H	6.39778574714411	22.90385777455532	7.89512880231842
H	12.85064303326284	17.45114199207455	7.85597217933946
P	13.56188079757459	12.45764733228849	8.08631387626916
H	7.70321980821153	4.53002828698417	2.61196077085676
H	7.70321989709469	20.84237166630933	2.68056180262654
H	7.70322005983099	15.40326654590253	2.65531098742131
H	7.70321994220675	9.95986320291710	2.62421712198191
H	3.85161004820394	15.39798400175415	2.64793616130655
H	3.85160995019421	9.96381137226852	2.62972784678484
H	11.55483006343723	15.39798442568061	2.64793742382766
H	11.55482988268158	9.96381194830063	2.62972866426765
H	2.55450152508554	17.25642176979785	3.96807765946527
P	1.92087903874994	12.29370951622785	3.98977938408212
P	9.62112886871972	17.72244984456839	4.00394749040659
P	9.64472932402091	12.29902575446378	3.98253244333746
P	9.63675431243064	6.85113827504188	3.95509838150205
H	9.01939446081483	22.71684277062405	4.00420264534404
H	0.63926650899765	14.47657184568818	5.89317724143022
H	14.76717406901419	14.47657318340526	5.89317634043141
P	7.70406348634511	4.06250517649968	5.85642886375241
P	7.70262817637790	20.48046611160122	5.90387508501264
P	7.70489458537565	15.01863182323390	5.88233110685022
P	7.69944522820413	9.61610322512998	5.85783494499946
H	4.48384897391726	19.92840928318719	5.92900073558040
P	3.87697277603079	15.02735613413813	5.88943957569639
P	3.80509509701098	9.56442489635150	5.88610763634333
H	10.92259262787518	19.92841060081648	5.92900142540360
P	11.52426124408868	15.03096696180409	5.89021598858458
P	11.60153103401820	9.56239809543004	5.87827150985893
H	2.55579665202190	17.45114111733178	7.85597169240729
P	1.83412966021817	12.44478445643284	8.09265280310226
P	9.59142163683382	17.88215596188682	8.10714254527337
P	9.65824431955979	12.39469774084927	8.01819541723352
P	9.67015520678859	7.00315325763734	7.99348426700375
H	9.00865315191435	22.90385832259270	7.89512910391923
C	6.19212294023905	10.77382091383354	11.07230578000696
C	6.33796562694101	9.83712115388280	10.12380073153619
C	8.76821470198477	9.92874020308088	10.35879973123617
C	8.57487038224809	11.22860974590365	11.09871908170091
C	7.33302183319726	11.60620262116428	11.45118320211212
H	7.15731821646986	12.51221266136495	12.02233600004032
H	9.45428979998741	11.79744143519964	11.37763281511565
H	8.83123168996560	9.08514448501426	11.06136761217334
H	5.54789772887777	9.20176815035451	9.74643155257824
H	5.22403564905490	10.92824814375129	11.53457420297422
N	7.60876696203296	9.71039384926457	9.44068121640349

H	7.68248457091465	8.76873056433446	9.05576532731784
H	9.67682192288204	9.93250413463810	9.75444969739337

Adsorbed PyH⁺

Energy=-8514.81284065691

H	5.77741514210618	18.48719914061344	2.80454892211872
H	5.77741499457454	13.04046331441147	2.76833017621631
H	5.77741484460623	7.59242000523336	2.73413671809092
H	13.48063510313242	13.03905261443101	2.77042345233472
H	6.55859719647575	3.22350858837736	5.83627545780902
Ga	5.80251018441845	19.12068873340959	5.98422889565173
Ga	5.78979520254926	13.64642145967214	6.00971762404715
Ga	5.79287264781780	8.25525009246018	6.00140111691432
Ga	13.45523847393703	13.69717523989300	6.03442281603061
H	12.70392623988963	8.66726201681755	5.87242505858612
H	1.92580493836109	13.03905178152976	2.77042463459758
H	9.62902513361281	18.48719928775240	2.80454878774509
H	9.62902506810481	13.04046294313389	2.76833073922744
H	9.62902498875347	7.59242090897887	2.73413542595681
H	0.77682476202635	11.44172606186044	3.92960751196675
H	14.62961393621505	11.44172599856829	3.92960799276114
Ga	7.70132044463341	16.34796378196093	3.87915736632897
Ga	7.70298448912609	10.90663469634568	3.86746128466524
Ga	7.70347352717669	5.41967531505075	3.85343760700512
Ga	7.70318604898975	21.84280285657803	3.88804213066290
Ga	3.82704301893616	16.35219809656095	3.87881480133137
Ga	3.84100990942727	10.88810197996448	3.86002946329711
H	4.62962033243677	5.99564063259968	3.89357729006170
Ga	11.57723553748035	16.35640426239642	3.87537964017751
Ga	11.56554383077224	10.88777929875637	3.86065594786642
H	10.77682037643929	5.99563932919888	3.89357704061201
Ga	1.94444492879416	13.68889279284878	6.03919251781043
H	2.70251336029371	8.66726128226904	5.87242543409418
H	8.84784154169556	3.22350885991058	5.83627575151047
Ga	9.60347581896329	19.12137963780435	5.98370596928372
Ga	9.61674234339954	13.65285028675748	6.00336887407981
Ga	9.61548194533191	8.25399269497001	6.00071811023280
H	0.74235904525402	11.64697401925667	7.64093316459997
H	14.65193831672592	11.67486479311455	7.61113872725639
Ga	7.70344356209424	16.66542829530277	7.52974482742312
Ga	7.71136809203176	11.01605222492145	7.88043683536251
Ga	7.70316206914671	5.80075755656991	7.57796555060755
Ga	7.70321504153366	22.19025767746071	7.44481248769657
Ga	3.90898021932512	16.72506796831096	7.48734071679963
Ga	3.77114757447486	11.24529085927287	7.57486366600594
H	4.60139065542767	6.22734720391853	7.60533343587441
Ga	11.49608495710789	16.72823675173316	7.48638032979289
Ga	11.62823217420454	11.25014815022043	7.57706193420012
H	10.80504989196189	6.22734630874561	7.60533302559530

P	5.78412488717677	17.71929544091856	4.00355943152294
P	5.76652723295581	12.29791369919359	3.98395955982369
P	5.76839500754164	6.85677739453855	3.96292731145038
H	6.38704570885248	22.71684341991050	4.00420318196955
H	12.85194063755709	17.25642355988299	3.96807757012421
P	13.48182437011403	12.29092806102762	3.98952866306687
P	5.81174255492867	17.87802405459873	8.10409569016736
P	5.75359460152152	12.38586224894780	8.02576278573241
P	5.71621271675165	7.01297667971490	8.02943671229308
H	6.39778592927214	22.90385778863621	7.89512875509073
H	12.85064302762660	17.45114199618414	7.85597218013340
P	13.56356608417681	12.45700763590397	8.08854638927027
H	7.70321981356448	4.53002827152746	2.61196073612892
H	7.70321995164224	20.84237179921262	2.68056192871090
H	7.70322004863701	15.40326656472070	2.65531104390964
H	7.70321991963668	9.95986321923835	2.62421707324339
H	3.85161004165009	15.39798398916940	2.64793613066940
H	3.85160995155770	9.96381135316305	2.62972783049807
H	11.55483004159037	15.39798440421867	2.64793740526564
H	11.55482986024960	9.96381192539165	2.62972871757847
H	2.55450151528952	17.25642177642720	3.96807768041404
P	1.92435330660565	12.29034705868809	3.98914156807064
P	9.61992282829010	17.71956760956498	4.00321648037881
P	9.63989503709186	12.29814632429000	3.98392480690600
P	9.63835880062541	6.85636064270008	3.96231331675525
H	9.01939436142358	22.71684269396495	4.00420261142832
H	0.63926649994100	14.47657183776275	5.89317725240277
H	14.76717403925256	14.47657319993841	5.89317632903617
P	7.70313504740170	4.07236609383573	5.87855958587691
P	7.70288311376425	20.47840085901674	5.90386880734655
P	7.70127727132619	15.01341391785955	5.88648816740691
P	7.70581079782920	9.63425503959488	5.88441579971125
H	4.48384893353424	19.92840930533258	5.92900073403689
P	3.88253979217164	15.01664381446172	5.89352595513241
P	3.80829006702389	9.56027298013944	5.88983436654039
H	10.92259266723671	19.92841061948362	5.92900142085876
P	11.52018378868445	15.02491160240622	5.88862602278835
P	11.59865106813355	9.56188307472353	5.89131706178599
H	2.55579667485500	17.45114111144651	7.85597167926304
P	1.83275445821232	12.44392078153125	8.09299391984945
P	9.59347916049869	17.87998416477079	8.10476445186064
P	9.65121469913984	12.40244607629326	8.02263291001977
P	9.68998397253952	7.00990102466000	8.02574804559826
H	9.00865298528591	22.90385826345225	7.89512907753069
C	6.56415935277450	8.79879195504645	11.31473883099272
C	6.60420623160349	9.56542922645228	10.18009644149790
C	9.02736384099949	9.69506890080319	10.22650228752980
C	8.97072125723663	8.49543276463259	11.14714986155623
C	7.79618033975238	8.14514462064487	11.71375072057006

H	7.75209327053012	7.31961368643009	12.42323790021849
H	9.89336963840905	7.96335189797431	11.35996780350486
H	9.82062688451655	9.56272522076882	9.48000502533641
H	5.68055703394824	9.90253713000777	9.71251445231217
H	5.61309199714084	8.52424578651735	11.75706596287051
N	7.74471897954596	9.90846839595656	9.51695323830637
H	9.29684716805582	10.60977989165546	10.79492494911825

8) H₂O pK_a

H₂O solvated by 2 H₂O

Energy=-229.212018822445

O	-2.43544394907979	-0.20947738261728	-0.11808683230471
H	-1.74716960266861	-0.03798006476703	-0.80150246286949
H	-2.87244636626946	0.64791430571056	-0.01328028021905
O	-0.04867439656405	0.32675217551541	-1.40911093844062
H	0.22717725104905	0.27582503565648	-0.46773030948981
H	0.26594843375366	-0.50384590386673	-1.79266347328365
O	-0.11201604896076	0.05621970062857	1.37209202985680
H	-1.04303103004413	-0.07826421512461	1.08413867464696
H	-0.09182991121592	0.97522203386465	1.67554667610356

OH⁻ solvated by 2H₂O

Energy=-228.703147576052

O	-2.48740515667120	-0.21731414421056	-0.39747836444225
H	-1.61023214914939	0.00736322689570	-0.91308578803939
H	-2.69467877226745	0.62092838876017	0.03771810308757
O	-0.24437749547309	0.32931083008078	-1.49968579313310
H	0.06513470131531	0.30677880474056	0.08332798391345
H	0.07624751641759	-0.56599769267339	-1.68272918171805
O	0.01574909824573	0.17461058397595	1.09037002162118
H	-0.88651494138789	-0.17874275852322	1.13500591807263

9) o-DHP pK_a

o-DHP solvated by 1 H₂O

Energy=-325.71730974562

C	-3.30897847048301	-0.15826260199361	-3.24748732687337
C	-1.79809254375148	-0.10677764702961	-3.35799321346776
C	-1.78679894827950	-0.14349685617261	-0.91107894307886
C	-3.10791231777339	0.16520513374043	-0.83697269418324
C	-3.90394364018905	0.02796988381661	-2.05166933437224
H	-4.98950852700457	0.04076865307122	-1.97191418056553
H	-3.56875718638018	0.41096214580555	0.11272164965523
H	-1.14704964011895	-0.17107065040782	-0.03338486364243
H	-1.44152468617129	-0.76307182324599	-4.15874745938768
H	-3.88563791506041	-0.29574451078644	-4.15768947512817
N	-1.19074760830082	-0.55045406959807	-2.08949277567737
H	-0.17030208460135	-0.50075703554300	-2.08916098456289
H	-1.46556235432967	0.91698263316302	-3.62480001945291
O	1.71565322703491	-0.19086545961276	-2.21685386275019

H	1.83523277225485	-0.44507240084088	-3.14314793221702
H	1.72386574453777	0.77657150983812	-2.24213931291720

PyH⁺ solvated by 1 H₂O

Energy=-325.204871690958

C	-3.25087888277327	-0.11263789372802	-3.36069701580621
C	-1.75594882557301	0.13793093021857	-3.40444369085569
C	-1.71664869611600	-0.20375358200533	-1.07792173334895
C	-3.05688133379371	0.17079954345350	-0.95786681018633
C	-3.85680167015288	0.01637609361170	-2.15027103346653
H	-4.93858571737628	-0.09398017610444	-2.05311047829251
H	-3.52106670760316	0.25152814767503	0.02144323011950
H	-1.14854654703214	-0.43048942834160	-0.16954743437444
H	-1.30773830612360	-0.28201049703138	-4.31402749702772
H	-3.80026258591633	-0.36608911700183	-4.26509058551634
N	-1.06401177632142	-0.43073977574157	-2.22576227652975
H	-1.55562587248725	1.23541992716132	-3.44751187442240
O	1.48488112639858	0.40850741381847	-2.13880318479274
H	0.53849905559456	0.04822874519506	-2.20278480736724
H	1.36050781913027	1.25551809258710	-1.69034086120966

Proton coverage effect on adsorbed proton acidity (see Figure S6 for proton numbering)

1) Adsorbed H₁⁺*

Same structure as in previous section

2) Bare cluster

Same structure as in previous section

3) Co-adsorbed H₁⁺* and H₂⁺*

Energy=-8266.834988543254

H	5.77741507744460	18.48719913977761	2.80454886640194
H	5.77741500437873	13.04046332106745	2.76833021864616
H	5.77741491817657	7.59242008153504	2.73413664388531
H	13.48063521694274	13.03905258006883	2.77042341085747
H	6.55859749274503	3.22350853807286	5.83627542886544
Ga	5.80277770517485	19.13940783781910	5.96370324329774
Ga	5.75868950549278	13.70834012008432	5.85815162845057
Ga	5.75436676259428	8.20329239184952	5.98423114279170
Ga	13.49356452110634	13.65400046829601	6.02532204890726
H	12.70392626800551	8.66726182376265	5.87242509760991
H	1.92580487246483	13.03905168348478	2.77042468828294
H	9.62902521364390	18.48719939754862	2.80454887859172
H	9.62902507366895	13.04046298586711	2.76833078604233
H	9.62902487207543	7.59242103655169	2.73413538238730
H	0.77682482040077	11.44172613819043	3.92960746027952
H	14.62961379708568	11.44172599320556	3.92960802872165
Ga	7.68626544573306	16.37397526958402	3.84586209977299
Ga	7.72473422070119	10.93330542708880	3.82035275550861
Ga	7.70268957051991	5.40069509443873	3.85568889423159
Ga	7.70180014740544	21.86144212750999	3.86626739687427
Ga	3.81581668187290	16.36606877770041	3.85646312709624

Ga	3.79429957955096	10.89307036694926	3.83431621996272
H	4.62962025589704	5.99564054086143	3.89357730065686
Ga	11.59405313572072	16.36860614959937	3.84267165316147
Ga	11.59473986803650	10.88446860966772	3.84853456495555
H	10.77682054959250	5.99563917921865	3.89357707472235
Ga	1.93410085454622	13.68783750214229	6.03054868837681
H	2.70251341840671	8.66726132460284	5.87242544213412
H	8.84784125470863	3.22350891153359	5.83627573443994
Ga	9.59255224470103	19.17469652073526	5.85271002600407
Ga	9.63918627003081	13.66266752462284	5.99010376034931
Ga	9.67315788588171	8.20026908480445	5.96815088023425
H	0.74840068359165	11.67346249399800	7.64098895028880
H	14.65803974852143	11.67346255442087	7.64098959922702
Ga	7.51216368259626	16.58810080378420	7.55351212934778
Ga	7.88079012229749	11.12349628464143	7.50934848392241
Ga	7.70705761689032	5.76973520528935	7.57376265318252
Ga	7.70387338235417	22.20857053826767	7.45031351817038
Ga	3.90235516576284	16.75619041132350	7.51195678979630
Ga	3.58974068262576	11.12888124021567	7.58950801495932
H	4.60139090867076	6.22734727311987	7.60533347751252
Ga	11.61789255818707	16.62357231717836	7.46937506451389
Ga	11.68969108873300	11.20925631752553	7.58203385909480
H	10.80504969325973	6.22734634288680	7.60533301741266
P	5.77517103558809	17.72330897800654	4.00463014434476
P	5.75487562787449	12.26936298960133	3.95698410459139
P	5.77154969128937	6.84445217589889	3.95130861111894
H	6.38704585111038	22.71684329065288	4.00420317680790
H	12.85194065261034	17.25642358306135	3.96807750597176
P	13.48947000115253	12.28962120266167	3.98371970373694
P	5.78042464480667	17.93583764301763	8.14394010617286
P	5.74841002984716	12.15861687009901	7.75444574253649
P	5.72612056068791	7.00460238416771	8.01821900955344
H	6.39778584210111	22.90385778037203	7.89512878570179
H	12.85064304633001	17.45114200089554	7.85597218804378
P	13.57411235199199	12.46673519985660	8.10393769181033
H	7.70321978040893	4.53002826237863	2.61196077224452
H	7.70321995211846	20.84237191794830	2.68056202551734
H	7.70322007729136	15.40326642077491	2.65531092800583
H	7.70321991790786	9.95986318460588	2.62421713570098
H	3.85161009259668	15.39798395291908	2.64793613727304
H	3.85160996005859	9.96381135151706	2.62972783895652
H	11.55483002099200	15.39798435751245	2.64793744575165
H	11.55482985649508	9.96381196628905	2.62972864919666
H	2.55450149405926	17.25642183970080	3.96807770294685
P	1.91169401270954	12.30003469771948	3.99002411276896
P	9.62145998795111	17.70151865268630	3.98093851209225
P	9.65641338399070	12.30027089588828	3.98420728795236
P	9.63468033918083	6.84033326901142	3.94780928039359
H	9.01939426271475	22.71684268723913	4.00420255805754

H	0.63926647187018	14.47657187718809	5.89317728048862
H	14.76717400898325	14.47657331128722	5.89317636111811
P	7.70318411688610	4.06489452911494	5.87606981193680
P	7.69260953955641	20.49352672107578	5.90440033103307
P	7.70167055995953	15.00544212189243	5.87196116999448
P	7.71509447917886	9.54754924310544	5.80430312751477
H	4.48384886333832	19.92840941010474	5.92900075469912
P	3.86461168448427	15.04187270088433	5.90999852807766
P	3.80153486861374	9.55346070073250	5.86152978677188
H	10.92259254381152	19.92841049294148	5.92900140541959
P	11.54902731208630	14.99190018291794	5.85146740069418
P	11.60564419731767	9.56293259713337	5.87874921698311
H	2.55579673693386	17.45114107474438	7.85597164928651
P	1.80911515079873	12.48772880163437	8.12300699367131
P	9.56872326361436	17.66118016923960	7.80279313869913
P	9.70708163916684	12.41327450006587	8.06591973366250
P	9.68184818210652	7.00956632903061	8.01156677748025
H	9.00865306702818	22.90385829965679	7.89512904342027
H	5.75741008729043	13.01610162026663	8.86669018632219
H	9.59244463348670	18.50474598607005	8.92431893237832

4) Adsorbed H₂⁺*

Energy=-8266.393493989219

H	5.77741508675827	18.48719916336944	2.80454887338602
H	5.77741497998394	13.04046332811589	2.76833018589366
H	5.77741496076361	7.59242013923418	2.73413663767946
H	13.48063516658387	13.03905262639730	2.77042339209197
H	6.55859744271023	3.22350855205189	5.83627542051885
Ga	5.79931413102945	19.12889530110528	5.97130563568135
Ga	5.75030118690279	13.65562389940799	5.97653586569122
Ga	5.74983231588370	8.22296022005213	5.97507914552792
Ga	13.48846747494190	13.65500649959812	6.02047531183005
H	12.70392623372971	8.66726184531831	5.87242508873867
H	1.92580486754037	13.03905174306316	2.77042459194038
H	9.62902520885989	18.48719939343329	2.80454887087134
H	9.62902506439016	13.04046298436550	2.76833079573799
H	9.62902485492635	7.59242106859900	2.73413536238002
H	0.77682476715568	11.44172606228556	3.92960748818065
H	14.62961385391612	11.44172593524119	3.92960803914459
Ga	7.67763257744739	16.35978456265543	3.85870907943747
Ga	7.69842765517552	10.92870014921812	3.83106692748924
Ga	7.70256686885623	5.40786034313994	3.85300029337996
Ga	7.70174271566605	21.85712308787139	3.87127582660959
Ga	3.81664024677369	16.35604874732716	3.86678689142898
Ga	3.81440694969518	10.88952550860344	3.84697721077878
H	4.62962019105067	5.99564048080987	3.89357730311485
Ga	11.59103096792576	16.36573309839737	3.84782264123303
Ga	11.57654932792917	10.88702586953053	3.85029895741177
H	10.77682057544692	5.99563915631103	3.89357708503796

Ga	1.93818664833801	13.68880140650841	6.04237903509735
H	2.70251351775997	8.66726146039052	5.87242546617507
H	8.84784131217825	3.22350889518723	5.83627573404203
Ga	9.59269615070714	19.16707351531079	5.85215753444492
Ga	9.62471656947429	13.65799468902021	5.99765465000839
Ga	9.65317539887018	8.22137592342930	5.97582742572475
H	0.74840053447111	11.67346243028511	7.64098894012327
H	14.65803974660160	11.67346255146733	7.64098960150863
Ga	7.50403847008672	16.57140155741893	7.54716817484125
Ga	7.69557305003082	11.20392369924939	7.49297525405114
Ga	7.70241229960966	5.77621837645036	7.57029760626620
Ga	7.70380304156217	22.20470840675147	7.44790669260932
Ga	3.89524710182378	16.73081346171434	7.50514857403704
Ga	3.74540964169866	11.21645041264043	7.56874383209461
H	4.60139089609667	6.22734725420284	7.60533348406364
Ga	11.61622054825594	16.62211377375346	7.46290764905513
Ga	11.65551591646713	11.21668856694378	7.56798926247765
H	10.80504969203855	6.22734634357361	7.60533301280476
P	5.77321835846106	17.72224398235725	4.00348591897045
P	5.75145294287908	12.29167143082114	3.97780680141763
P	5.77067897324491	6.84557164389413	3.95234627860315
H	6.38704578230555	22.71684332523346	4.00420318999011
H	12.85194065047547	17.25642358414789	3.96807752438624
P	13.48432219844037	12.28554927099710	3.98161376613306
P	5.77313952739766	17.92424627381753	8.13998166050150
P	5.74266325083425	12.37768895658910	8.02694075081373
P	5.72566905259131	7.00943458582565	8.01091461683056
H	6.39778591825884	22.90385777695506	7.89512877594702
H	12.85064304523867	17.45114200428589	7.85597218678270
P	13.55940586879858	12.45901480325568	8.09342076503777
H	7.70321978246749	4.53002825615314	2.61196079702310
H	7.70321995859768	20.84237188596615	2.68056200548426
H	7.70322007252605	15.40326641864524	2.65531094131713
H	7.70321991328606	9.95986317877161	2.62421712491417
H	3.85161013152957	15.39798387758230	2.64793607458650
H	3.85160997230848	9.96381132120930	2.62972782693052
H	11.55483001554774	15.39798434705902	2.64793742558949
H	11.55482986888802	9.96381196953999	2.62972867819223
H	2.55450141232434	17.25642191119648	3.96807772292611
P	1.91715863986308	12.29729447852878	3.99051144732888
P	9.61590179025357	17.69666619216633	3.97845320327341
P	9.64287330237236	12.29868834090394	3.98360974615097
P	9.63531737954484	6.84507662149342	3.95201978401460
H	9.01939431912827	22.71684270742583	4.00420257037448
H	0.63926669596545	14.47657184405326	5.89317737414401
H	14.76717401338811	14.47657331477800	5.89317636097994
P	7.70316668223634	4.06650982539034	5.87339888718272
P	7.69095272335807	20.48782124879921	5.90537328597407
P	7.68564825305394	14.99573454509209	5.86574917472716

P	7.70210831887768	9.55851496437447	5.81718489758319
H	4.48384888602154	19.92840937664340	5.92900076774435
P	3.87156309845619	15.03498533445390	5.89820392550946
P	3.80180915927265	9.56156158978590	5.87358721709968
H	10.92259258498736	19.92841051860200	5.92900141736218
P	11.54209296285501	14.98749374779913	5.84974389184298
P	11.60220279223890	9.55939456847972	5.87542264897577
H	2.55579667861855	17.45114110491644	7.85597167036709
P	1.84465056166613	12.45818116347344	8.09945179319709
P	9.56422707373983	17.65466163734154	7.80400766742259
P	9.65497009544724	12.37247981168212	8.03416511799251
P	9.67991750607281	7.00828422581437	8.01147439069423
H	9.00865298890794	22.90385828057305	7.89512903368244
H	9.59694931728410	18.50726020742736	8.91949648272930

5) Adsorbed $H_1^+ + 1H_2O-OH^*$

Energy=-8418.805400262951

H	-1.89126799901149	5.22936299793697	-3.08239700025302
H	-1.89129304034937	-0.21736701799186	-3.11949099033000
H	-1.89131802445038	-5.66540501222636	-3.15456000333634
H	5.81192801756389	-0.21877900763145	-3.12273899742760
H	-1.10798497346849	-10.03481499938603	-0.05366498437753
Ga	-1.86117238942657	5.87036515655365	0.09165421991822
Ga	-1.89564571990783	0.52290066893741	-0.06624238997598
Ga	-1.93216787974256	-5.00920520821975	0.09551619044415
Ga	5.79378658181553	0.43399657108441	0.14907158541035
H	5.03736900015177	-4.59106700596342	-0.02090000729960
H	-5.74290198098786	-0.21877800111923	-3.11472598329045
H	1.96034200357568	5.22936299294023	-3.08506699694072
H	1.96031700123928	-0.21736799653083	-3.12215999537200
H	1.96029199876923	-5.66540400614577	-3.15723099579318
H	-6.89107801999327	-1.81628999652390	-1.95500299993357
H	6.96171098522361	-1.81629198640199	-1.96460700490365
Ga	0.05472910439149	3.11336384647771	-2.02936834880199
Ga	0.04682247238971	-2.33199762153978	-2.04645858978789
Ga	0.02806592130584	-7.83875948524351	-2.04442489687397
Ga	0.03536485337232	8.58814189802593	-2.00374981262616
Ga	-3.84415286641621	3.11251682686942	-2.02632205119126
Ga	-3.85995019110080	-2.38372779657771	-2.01379299407097
H	-3.03830899921546	-7.26237000320226	-1.99458001208695
Ga	3.91173024402625	3.09270974886819	-2.01231482575423
Ga	3.91129727014196	-2.36569457200926	-2.03955061335046
H	3.10889199502511	-7.26237199314658	-1.99884199665471
Ga	-5.72706024029556	0.39765788458857	0.18142921649283
H	-4.96404284125257	-4.59106687061272	-0.01396703363168
H	1.18125897135636	-10.03481398567055	-0.05525200053365
Ga	1.93644500152022	5.87045230348729	0.09788674068903
Ga	1.94432215419123	0.38082264328467	0.13954607141863
Ga	1.96998325865702	-5.01915511396587	0.07965570736916

H	-6.91692904968954	-1.58514998963424	1.75643501579503
H	6.99270999711183	-1.58515199323382	1.74679199570035
Ga	0.03907277153387	3.42768487641700	1.64409953689680
Ga	0.06022720246093	-2.23303617078571	1.83195245646701
Ga	0.03495906904750	-7.49488454618280	1.64884941276996
Ga	0.03762667399679	8.93461931589938	1.55808631873515
Ga	-3.75284676508431	3.48821476144284	1.59847701683748
Ga	-3.97093801499231	-2.28471543293081	1.99719280842146
H	-3.06396403479936	-7.03126003928396	1.71723300140755
Ga	3.82940364119910	3.47210315870743	1.60560858525776
Ga	3.98524414798212	-2.04455242559082	1.70268568140408
H	3.13969401204545	-7.03126100336519	1.71293200355476
P	-1.87857052702016	4.46171173300556	-1.88450043388240
P	-1.91190690811423	-0.97432040589910	-1.92748244785853
P	-1.90237641954799	-6.40275887754489	-1.92932170656121
H	-1.28080399746502	9.45881399904281	-1.88248499867996
H	5.18406498957878	3.99839999486520	-1.92397099750727
P	5.81864229402775	-0.96290613910725	-1.90236847697655
P	-1.85165103301295	4.63005671544108	2.22222460931390
P	-1.94421571830876	-0.95483214060887	1.76634276228660
P	-1.92542403831606	-6.26893765757311	2.11076957970204
H	-1.26736699644934	9.64520400330727	2.00846299984494
H	5.18546299367120	4.19249400041954	1.96395599617090
P	5.89719501784828	-0.80110505816167	2.20655744530864
H	0.03440201015902	-8.72777699213631	-3.27856300186395
H	0.03445199880034	7.58455500106811	-3.20734100038055
H	0.03443300049421	2.14545400273304	-3.23346499443123
H	0.03441200032257	-3.29794402089066	-3.26543401768457
H	-3.81718100017248	2.14017400287263	-3.23817000126312
H	-3.81719499341634	-3.29399602559669	-3.25725198802511
H	3.88603900443741	2.14017300527374	-3.24351099323074
H	3.88602500285778	-3.29399599980811	-3.26259199927586
H	-5.11337399445631	3.99839899628825	-1.91683199668820
P	-5.74925892145766	-0.96200093111807	-1.89339968223574
P	1.96394218919876	4.47046695465988	-1.88449344010759
P	1.98010055260457	-0.95660407101383	-1.90129203434451
P	1.96692913662325	-6.41023783523196	-1.93805920068125
H	1.35154399955490	9.45881399874000	-1.88431100011212
H	-7.02727601673291	1.21824098322460	0.00914999437823
H	7.10063296625186	1.21823997838749	-0.00064699551818
P	0.03757514453128	-9.19502643839633	-0.03283733104013
P	0.03731760916211	7.22447188427847	0.01460964322093
P	0.05942000667803	1.78408701820380	-0.01304602020851
P	0.02466138184639	-3.67163233951309	-0.05681914481067
H	-3.18266700638631	6.67007200213207	0.04318399912758
P	-3.82631197389415	1.79512101718136	-0.00732781742954
P	-3.88310010355247	-3.66852341364411	0.02482200157675
H	3.25607699239005	6.67007199564361	0.03872000168570
P	3.84862420776594	1.75327089509486	0.01692738413109

P	3.93508859729755	-3.69546690560947	-0.00969306418098
H	-5.10938396706729	4.19249398962208	1.97109298538332
P	-5.80986382614883	-0.81799159535422	2.22232798317656
P	1.93056877186271	4.62933752369280	2.21948299961905
P	1.97973119337500	-0.91359550023582	2.19096609595357
P	2.00335981031087	-6.25570514267224	2.10593690041902
H	1.34349999645406	9.64520400110624	2.00665300115597
O	-3.28994959882798	-3.39831897152222	3.42067752349912
O	-0.71906895959820	-3.37011245393430	3.38513794986051
H	-1.90000138859368	-0.11763768068155	2.89888786963533
H	-3.55937864826182	-3.04926342076556	4.28518176178919
H	-1.76508888775130	-3.42229289860848	3.40998678736113
H	-0.36791198664062	-4.25838291460128	3.55532962886219

6) Bare cluster + 1H₂O-OH*

Energy=-8418.338940086251

H	5.77741507805338	18.48719918994189	2.80454893309095
H	5.77741488965237	13.04046332053683	2.76833024403240
H	5.77741490163875	7.59242005726281	2.73413664756212
H	13.48063524068133	13.03905249579488	2.77042348967508
H	6.55859728250576	3.22350850325964	5.83627544024733
Ga	5.80246547414623	19.12040662506480	5.98172436017318
Ga	5.75599662695585	13.69984418513645	5.94952022749375
Ga	5.73181654776568	8.27376302740760	5.98249605410118
Ga	13.45674381767187	13.69532219369747	6.04262126631036
H	12.70392627945885	8.66726175194360	5.87242510998989
H	1.92580487033090	13.03905174580388	2.77042460457405
H	9.62902516852102	18.48719932139144	2.80454883486225
H	9.62902505330035	13.04046303561584	2.76833078989530
H	9.62902483635024	7.59242103620336	2.73413537040242
H	0.77682479863239	11.44172609131711	3.92960749215337
H	14.62961374785669	11.44172615876519	3.92960795217213
Ga	7.71352651716753	16.35582711905100	3.87264221813619
Ga	7.69060862862783	10.92520627643112	3.84993647022379
Ga	7.69422553780052	5.42992326738551	3.83963275925895
Ga	7.70319690228223	21.84295823593549	3.88802223908081
Ga	3.82399303139966	16.36085901892217	3.86975766731323
Ga	3.82304381125836	10.87413196589082	3.87842926537549
H	4.62962028746962	5.99564056617097	3.89357729990235
Ga	11.57667081335527	16.34989173137383	3.88287856401584
Ga	11.56716374358424	10.89584458327719	3.85356693531169
H	10.77682054149343	5.99563919467311	3.89357707579574
Ga	1.94548066774034	13.66370828795601	6.07710911168102
H	2.70251354121694	8.66726146115065	5.87242544777899
H	8.84784143612986	3.22350887963851	5.83627573655494
Ga	9.60271320018747	19.12301087193991	5.98679613740330
Ga	9.59673897942766	13.64101885370513	6.03436263279643
Ga	9.61664790678340	8.26173515440633	5.98119035378168
H	0.74840063937880	11.67346247288949	7.64098896726193
H	14.65803976552582	11.67346263161466	7.64098960002608

Ga	7.69750797488025	16.66303345624703	7.51995450325526
Ga	7.57045375083666	11.13453707904620	7.70224789770347
Ga	7.69883952577129	5.76239067180588	7.52890439957412
Ga	7.70310028339387	22.19039263924732	7.44465168906962
Ga	3.90790636152089	16.72917263089947	7.47578080804495
Ga	3.83972436051875	11.08084908814150	7.84935589688941
H	4.60139086039768	6.22734722937130	7.60533348213117
Ga	11.49375178956790	16.72892013843858	7.49199530793350
Ga	11.62682102555450	11.22297089510649	7.58243932143987
H	10.80504968636491	6.22734637160684	7.60533301180229
P	5.78697271682186	17.71833074592966	4.00142396668476
P	5.75059405462491	12.29882471653739	3.97753811418234
P	5.76319043347355	6.85941160693507	3.96271441032201
H	6.38704561553342	22.71684346389989	4.00420321448614
H	12.85194066250951	17.25642361809088	3.96807757390071
P	13.48424848433269	12.29346123288645	3.99046227224132
P	5.81052233874532	17.87983269559538	8.10254754202982
P	5.71687538609826	12.53884872970319	7.95516538604953
P	5.74305648000324	6.98631418223711	7.98940601070801
H	6.39778612827514	22.90385780871561	7.89512871898352
H	12.85064296482345	17.45114199316995	7.85597214159549
P	13.55426136889175	12.45243246997964	8.09360032352106
H	7.70321981403482	4.53002833639724	2.61196081099299
H	7.70322003803033	20.84237178275948	2.68056194037533
H	7.70322006155296	15.40326650847428	2.65531100367092
H	7.70321995311135	9.95986306484850	2.62421701651180
H	3.85161005349129	15.39798402954577	2.64793624153857
H	3.85160999400388	9.96381134290088	2.62972784750427
H	11.55483003391979	15.39798434867958	2.64793738952658
H	11.55482987922017	9.96381199200438	2.62972869416984
H	2.55450150653591	17.25642177294105	3.96807761187645
P	1.92145332161752	12.29508867867853	3.99325862963378
P	9.62539524178194	17.72402711085234	4.00374414872423
P	9.63759463044428	12.30015304794814	3.98865066832925
P	9.63610705292000	6.85327683497642	3.95802623169654
H	9.01939435341790	22.71684268763564	4.00420261224924
H	0.63926654489099	14.47657187044848	5.89317727684279
H	14.76717397238931	14.47657311947741	5.89317635200029
P	7.70439372306058	4.06258839591494	5.85052212253930
P	7.70232686221104	20.47999347682173	5.90294752956115
P	7.70056968013141	15.02444538163737	5.86775519707899
P	7.67967952564478	9.61340106848305	5.84845027255620
H	4.48384900676888	19.92840927006330	5.92900073121512
P	3.85074991525408	15.04463188041249	5.86877127961083
P	3.78198118790732	9.60141891612961	5.91386149265078
H	10.92259263026883	19.92841059702628	5.92900143276263
P	11.51103967335364	15.01041471870743	5.90530362674817
P	11.59924366256373	9.55998721495147	5.88025907833426
H	2.55579671362825	17.45114108449071	7.85597164980046

P	1.87443289200625	12.42264180261289	8.09496866146406
P	9.58814159168744	17.87828688546036	8.10442565179189
P	9.61603629670019	12.32888766424549	8.06361870837617
P	9.66587264716894	6.99909989096266	7.99666968400403
H	9.00865278590895	22.90385820562664	7.89512904166045
O	4.36366579984319	9.80972352840936	9.24604240531333
O	6.92299522157607	9.86315561783922	9.24079846276739
H	4.10441299747973	10.16088141180636	10.11317167949899
H	5.87376630910763	9.80029950623096	9.26092875651947
H	7.26592542320713	8.95826116324367	9.30582676024036

7) Co-adsorbed H_1^+ and H_2^+ + $1H_2O-OH^-$

Energy=-8419.259261565247

H	-1.89126800516614	5.22936297947884	-3.08239700103482
H	-1.89129304701805	-0.21736700825470	-3.11949095214585
H	-1.89131802906769	-5.66540501462671	-3.15456000423859
H	5.81192802695980	-0.21877901098874	-3.12273900334355
H	-1.10798496624763	-10.03481499715342	-0.05366498219529
Ga	-1.86623779074878	5.87295759774791	0.07819402892952
Ga	-1.91566652534721	0.49136231056588	-0.07856390259577
Ga	-1.93284851934116	-5.01312783683718	0.09531552607738
Ga	5.81838972397284	0.39661476397796	0.13091765387490
H	5.03736900350073	-4.59106699760435	-0.02090000133139
H	-5.74290199465842	-0.21877799853732	-3.11472600270751
H	1.96034200517282	5.22936298293318	-3.08506698756214
H	1.96031703141294	-0.21736800660632	-3.12215999473653
H	1.96029198824541	-5.66540399527403	-3.15723099975277
H	-6.89107801600164	-1.81629000457492	-1.95500300273119
H	6.96171097491336	-1.81629197995421	-1.96460700432748
Ga	0.02825697007460	3.11610639531034	-2.04094824350313
Ga	0.04244214866914	-2.34030506304004	-2.04355072321397
Ga	0.02741193375353	-7.84005891490766	-2.04416420050324
Ga	0.03391451406590	8.60009078228730	-2.01776364360612
Ga	-3.85578953735069	3.10658427548497	-2.02797449858183
Ga	-3.87103110554414	-2.39160999575199	-2.01248270055494
H	-3.03830900041697	-7.26237000231522	-1.99458001098275
Ga	3.92590890158673	3.09469350164229	-2.03131140601584
Ga	3.90866078634243	-2.37529286875635	-2.03507559687535
H	3.10889201259289	-7.26237200893342	-1.99884199722806
Ga	-5.73292040273311	0.39314888043237	0.18449562297964
H	-4.96404285042921	-4.59106689532736	-0.01396705287807
H	1.18125896374659	-10.03481398203636	-0.05525200054785
Ga	1.92655236894549	5.91059122997914	-0.03622585728261
Ga	1.93127811804879	0.34471840102037	0.14857029266127
Ga	1.96832397418056	-5.02520125440011	0.08065105807491
H	-6.91692901479640	-1.58514999108853	1.75643502488118
H	6.99270998797496	-1.58515199048752	1.74679199747657
Ga	-0.15550494708065	3.33006409384868	1.65136413894392
Ga	0.05417555075910	-2.24323228460762	1.84462321395470

Ga	0.03429089513486	-7.49775465551204	1.65034720056896
Ga	0.03830398080530	8.94621594234535	1.56064015477043
Ga	-3.77165275893670	3.48111337945301	1.60311539092381
Ga	-3.97738665316929	-2.28882351184740	2.00127268767055
H	-3.06396402674450	-7.03126003437774	1.71723299997188
Ga	3.95553588538607	3.35281247978835	1.57021773838423
Ga	3.98802215177868	-2.05084422489125	1.70908194673132
H	3.13969400311504	-7.03126100077437	1.71293200553535
P	-1.89104312773757	4.46164279612739	-1.88556615660707
P	-1.91853845784278	-0.98721977978831	-1.93689879778423
P	-1.90225333924757	-6.40335861806952	-1.92984814444564
H	-1.28080399756638	9.45881399889657	-1.88248499953279
H	5.18406498385491	3.99839999562163	-1.92397099872760
P	5.81573898851279	-0.97292552229116	-1.91048891092871
P	-1.89428265603569	4.66694722088947	2.25316863783848
P	-1.94726861219662	-0.95892456971974	1.76935132007305
P	-1.92531949673836	-6.26928439204167	2.11148969227318
H	-1.26736699025427	9.64520400317550	2.00846299782204
H	5.18546299031756	4.19249399800836	1.96395598915461
P	5.89744614068836	-0.79972076778502	2.20455808578128
H	0.03440201015433	-8.72777699359161	-3.27856300350227
H	0.03445199850709	7.58455500495361	-3.20734099669490
H	0.03443300121995	2.14545401666369	-3.23346499499523
H	0.03441200821600	-3.29794402895573	-3.26543404768336
H	-3.81718102015477	2.14017403155633	-3.23816999400875
H	-3.81719498837380	-3.29399602668255	-3.25725195528409
H	3.88603900781915	2.14017299952110	-3.24351100408879
H	3.88602499085031	-3.29399598366061	-3.26259198722287
H	-5.11337395137681	3.99839896113139	-1.91683200193833
P	-5.75062399110176	-0.96107257776810	-1.89305625006542
P	1.95895388093859	4.44372489802644	-1.91092037549097
P	1.97529672630586	-0.96255157342540	-1.90463197092046
P	1.96641156709270	-6.41116796552297	-1.93872677894414
H	1.35154399735895	9.45881399783589	-1.88431100046351
H	-7.02727604432052	1.21824102774486	0.00914998245436
H	7.10063296043750	1.21823997397619	-0.00064699996607
P	0.03749741466731	-9.19546482773956	-0.03251631842093
P	0.02496215076968	7.23005038226474	0.01723664579298
P	0.04368635855066	1.76017272238541	-0.03351997512410
P	0.02443917413031	-3.67227965412319	-0.05195715292830
H	-3.18266700893902	6.67007200903327	0.04318399549432
P	-3.82569841392638	1.79394947630142	-0.00505270686459
P	-3.88297357560127	-3.66994366024840	0.02694712649661
H	3.25607698868621	6.67007199247619	0.03872000464642
P	3.85263585480598	1.70329451843056	-0.02768615093422
P	3.93305275124897	-3.69842348724354	-0.00528243000397
H	-5.10938396190093	4.19249398142376	1.97109298428558
P	-5.81156830486697	-0.81835711113101	2.22631210482828
P	1.90673565130816	4.39946093782113	1.91501602540275

P	1.97727982920537	-0.91897909295430	2.19996872488875
P	2.00268271841347	-6.25734413945710	2.10774027402785
H	1.34349999063080	9.64520400176910	2.00665300221711
O	-3.28186278022491	-3.39460331938659	3.42431169207036
O	-0.72179433256130	-3.37000425744208	3.39238580319541
H	-1.90485253734763	-0.10652022418586	2.89020280744324
H	-3.56339080710479	-3.05858106876476	4.29010210282690
H	-1.77286832608446	-3.41937429404815	3.41997932402543
H	-0.37354480799807	-4.25943648529374	3.56315451032968
H	1.93699902034071	5.25227574742203	3.03024933957972

8) Adsorbed $H_2^+ + 1H_2O-OH^+$

Energy=-8418.796641708221

H	-1.89126801527399	5.22936302053853	-3.08239704212979
H	-1.89129306992830	-0.21736707343915	-3.11949097556549
H	-1.89131802658456	-5.66540501189237	-3.15455999627295
H	5.81192798907973	-0.21877900338994	-3.12273899663905
H	-1.10798497615051	-10.03481499678812	-0.05366498328267
Ga	-1.87042448374734	5.86156995748537	0.08622543813682
Ga	-1.93205744939142	0.40437839505079	0.04863427343078
Ga	-1.93585013117176	-4.98769727394922	0.09397147856305
Ga	5.81470638320336	0.39841931976429	0.12798234489773
H	5.03736902328573	-4.59106702136136	-0.02090001313475
H	-5.74290195670802	-0.21877803060304	-3.11472594358474
H	1.96034201424754	5.22936301461136	-3.08506700439812
H	1.96031700140674	-0.21736801512071	-3.12216001664673
H	1.96029199718092	-5.66540400443931	-3.15723099417761
H	-6.89107802486751	-1.81628998341267	-1.95500300919189
H	6.96171100994932	-1.81629199705972	-1.96460700395855
Ga	0.01807753144311	3.09958151313552	-2.02676916101414
Ga	0.01908989613966	-2.34233131217442	-2.03701744096340
Ga	0.02656791423760	-7.83114034702205	-2.04854014122016
Ga	0.03390943372880	8.59557833685706	-2.01228620463092
Ga	-3.85499594076256	3.09698315661213	-2.01815982336726
Ga	-3.85431533846490	-2.39337596588495	-2.00603671052873
H	-3.03830899495207	-7.26236999951798	-1.99458000972457
Ga	3.92216360171000	3.09442420038430	-2.02811343801319
Ga	3.89424102345088	-2.37275687204641	-2.03383193090587
H	3.10889199076689	-7.26237199057912	-1.99884199553726
Ga	-5.72699187893108	0.39905252359512	0.19259498096971
H	-4.96404283637049	-4.59106686359802	-0.01396703513382
H	1.18125897547169	-10.03481399084378	-0.05525200296115
Ga	1.92660727139318	5.90228562579726	-0.03524058238246
Ga	1.91802998066470	0.34970625416214	0.15091265736538
Ga	1.94815577164921	-5.00111875128180	0.09127668315739
H	-6.91692901200146	-1.58514995158400	1.75643502086859
H	6.99270998367409	-1.58515198350091	1.74679199871108
Ga	-0.16930507971374	3.29792040709933	1.64134341500467
Ga	-0.10106851707167	-2.13009549797905	1.82402007557649

Ga	0.03264881536325	-7.49720229915045	1.64110829222056
Ga	0.03842397836758	8.94228778840828	1.55943936550787
Ga	-3.77909915321257	3.45767724094444	1.59302995773613
Ga	-3.83240006982298	-2.17956390647099	1.97206064762868
H	-3.06396404309109	-7.03126004661922	1.71723300118253
Ga	3.95378099996924	3.35293113752204	1.56573091351440
Ga	3.96426662968584	-2.04038176103613	1.69696314644566
H	3.13969401028387	-7.03126100117157	1.71293200152452
P	-1.89332975161540	4.46065312794104	-1.88634278942900
P	-1.92313778891504	-0.97343287136038	-1.92015549884939
P	-1.90409761300123	-6.39919744222612	-1.92655937744933
H	-1.28080398951373	9.45881400407450	-1.88248499957332
H	5.18406501827490	3.99839997086486	-1.92397095421872
P	5.81201441079575	-0.97591921962389	-1.91163515970764
P	-1.89931955355434	4.65319304197345	2.24410153225176
P	-1.95105333791158	-0.71977723024457	2.07150124995732
P	-1.92190180413379	-6.27208303589786	2.10194728724760
H	-1.26736698821585	9.64520400772322	2.00846300031268
H	5.18546318258188	4.19249417108803	1.96395616884402
P	5.88966955113832	-0.80350340342010	2.19740878103068
H	0.03440201226339	-8.72777698730841	-3.27856299813683
H	0.03445199659479	7.58455500698008	-3.20734099602152
H	0.03443299188429	2.14545398805529	-3.23346500306841
H	0.03441201709293	-3.29794400990809	-3.26543406410045
H	-3.81718100469228	2.14017403978892	-3.23816994794405
H	-3.81719498112910	-3.29399603080677	-3.25725203229064
H	3.88603895562656	2.14017293908964	-3.24351116229471
H	3.88602500238732	-3.29399599204804	-3.26259199324542
H	-5.11337397059462	3.99839897328150	-1.91683201883663
P	-5.74651453141805	-0.96332119975590	-1.89245121867821
P	1.95188904179461	4.43861417535156	-1.91280750942314
P	1.96475872534662	-0.96359975393160	-1.90525140342223
P	1.96742904501930	-6.40527034565595	-1.93367611331179
H	1.35154399097749	9.45881400025063	-1.88431099910381
H	-7.02727609887166	1.21824099132010	0.00914997988800
H	7.10063293668722	1.21823996345884	-0.00064699446626
P	0.03773182613013	-9.19516324911771	-0.03855215368514
P	0.02302393486503	7.22446611447577	0.01888189962027
P	0.01696690381455	1.73757926383831	-0.04500580600915
P	0.01212087678009	-3.64524030062475	-0.03507694418582
H	-3.18266697996179	6.67007197320876	0.04318400112438
P	-3.81500498847045	1.78171651810436	-0.01728650051770
P	-3.88494916877619	-3.65669561908911	0.03196038788437
H	3.25607690928717	6.67007191071783	0.03872001304198
P	3.84974350879716	1.70288205992860	-0.03075702915480
P	3.93110277461929	-3.70009510794525	-0.00693319767355
H	-5.10938401668885	4.19249400970119	1.97109299779719
P	-5.79298860334209	-0.83417566245749	2.21347907950408
P	1.89662337825857	4.38582577910767	1.91285402698508

P	1.94917051000971	-0.93490543172038	2.18061519109498
P	2.00001282510994	-6.26054820050111	2.10704402450877
H	1.34349998884552	9.64520400463274	2.00665300443201
O	-3.30034221191946	-3.44907865896509	3.36426083605435
O	-0.74742447418649	-3.39305718935330	3.35975055985553
H	-3.56644803411787	-3.10715801153791	4.23301760990134
H	-1.80052670926502	-3.45996738480265	3.38174884253938
H	-0.39855048704465	-4.29506856143601	3.43268389013526
H	1.93189313225086	5.24392554280572	3.02490881780289

9) Adsorbed $H_1^+ + 2H_2O - OH^-$

Energy=-8571.191777362435

H	5.77741508410294	18.48719915370216	2.80454893080720
H	5.77741496290952	13.04046339605236	2.76833020105426
H	5.77741494383911	7.59242009749046	2.73413665150674
H	13.48063509420357	13.03905259894920	2.77042343972361
H	6.55859732767132	3.22350849219336	5.83627542988664
Ga	5.79513100566732	19.11108585826107	5.97576184366222
Ga	5.74798913194057	13.83433926883024	5.82079360473365
Ga	5.73054458853126	8.25790806627269	5.98487619885599
Ga	13.45156305228149	13.70080232586118	6.03700023985052
H	12.70392629112770	8.66726173079915	5.87242508511187
H	1.92580497817207	13.03905184809953	2.77042456318804
H	9.62902511311526	18.48719932294999	2.80454883959251
H	9.62902505818503	13.04046307859383	2.76833077821847
H	9.62902483170368	7.59242105138042	2.73413536085399
H	0.77682472065920	11.44172600389098	3.92960755160122
H	14.62961387322819	11.44172602289409	3.92960799226536
Ga	7.71519196559450	16.36610285162929	3.87678966321535
Ga	7.70297557497021	10.93928829979269	3.83711405825957
Ga	7.69451869985392	5.42208269468417	3.84469308961515
Ga	7.70803132684796	21.83833446058667	3.89420463363796
Ga	3.82515871409596	16.35509992731692	3.89196032533258
Ga	3.80756481536778	10.89001147558052	3.86714819260830
H	4.62962024662854	5.99564053875999	3.89357731091064
Ga	11.56731069326504	16.35471756429989	3.88525734132134
Ga	11.56708086132740	10.89857226893068	3.85227976354981
H	10.77682055947052	5.99563918362258	3.89357708016378
Ga	1.98254946988162	13.71100036043651	6.08564414934705
H	2.70251342379206	8.66726132642086	5.87242543717650
H	8.84784138498089	3.22350892158811	5.83627573215313
Ga	9.59435552607786	19.10420347709914	6.03675616996520
Ga	9.56366912519466	13.68148068815674	6.02989907208083
Ga	9.63570686304724	8.24372240936364	5.96920904247549
H	0.74840065218905	11.67346249824361	7.64098897015076
H	14.65803972454784	11.67346262253493	7.64098961106932
Ga	7.58684868750793	16.60322435088484	7.75122048663669
Ga	7.70391273209117	11.03022978281764	7.70621666083053
Ga	7.69915593149260	5.76669655955275	7.53639846662492

Ga	7.70276280771015	22.18275447853364	7.43075168556735
Ga	3.96273989081499	16.61668306251020	7.81720358525817
Ga	3.68802672674180	10.98582766665713	7.86522497688665
H	4.60139090892534	6.22734727086872	7.60533347768866
Ga	11.48227682926032	16.72499489413865	7.51947155722849
Ga	11.63556987971648	11.23397659433402	7.59064819630131
H	10.80504968582533	6.22734636405010	7.60533301818499
P	5.78487409714841	17.71918884200526	3.99796557572983
P	5.75119667344766	12.30025440284924	3.97033009625431
P	5.76420205314703	6.85703430275431	3.96098095012521
H	6.38704550171048	22.71684348014348	4.00420321205270
H	12.85194062646810	17.25642353558981	3.96807752378277
P	13.48441823793012	12.29390384222191	3.99048866276974
P	5.80215813476710	18.05157001327548	8.05762999357571
P	5.70418191149203	12.29859154094362	7.61709226127494
P	5.73916783991843	6.99173504527987	7.99825851721417
H	6.39778613640922	22.90385788991048	7.89512873806110
H	12.85064294653971	17.45114201766632	7.85597213045162
P	13.56047662971173	12.46164007611486	8.09500604841760
H	7.70321979800192	4.53002828141919	2.61196079608319
H	7.70322007974997	20.84237174737800	2.68056190982912
H	7.70322007982621	15.40326648924726	2.65531097865090
H	7.70321992507025	9.95986304143199	2.62421706230582
H	3.85161004540866	15.39798401098960	2.64793619118038
H	3.85160996742449	9.96381132986677	2.62972787132653
H	11.55483007168100	15.39798444618877	2.64793745537706
H	11.55482989612148	9.96381195142926	2.62972870367662
H	2.55450152963631	17.25642176864300	3.96807766075277
P	1.91427201484409	12.30836456537835	4.00188457249861
P	9.62510328968849	17.73283886490399	4.01187149682946
P	9.63980015736110	12.31164817457888	3.99621381674125
P	9.63505110626217	6.84814651361790	3.95366996666790
H	9.01939439719825	22.71684271812647	4.00420262649016
H	0.63926644690258	14.47657187467914	5.89317726329997
H	14.76717413057581	14.47657323008707	5.89317634963462
P	7.70402407569993	4.06374462687992	5.85659493685005
P	7.70500061438320	20.48008543458039	5.88563958814058
P	7.70011256668323	15.10196591620573	5.90388381838900
P	7.69087579541945	9.58694919943271	5.82479594932665
H	4.48384901840698	19.92840928769390	5.92900071886064
P	3.84812086012199	15.13326614823889	5.92241744001830
P	3.77837572109533	9.59298921485276	5.90463717247395
H	10.92259275195203	19.92841052131217	5.92900142838977
P	11.50576769922078	15.01109654113527	5.91537555434359
P	11.60101232575032	9.56664753700618	5.88376576095744
H	2.55579663517571	17.45114110327857	7.85597167954443
P	1.85060575874005	12.44771847906679	8.11081567327634
P	9.56891325593503	17.83974543441531	8.13672173509306
P	9.61883614463012	12.35667209349029	8.07808622197355

P	9.66801665603538	7.00413130466855	7.99523701196155
H	9.00865277302971	22.90385815869051	7.89512905464119
O	4.37827355969422	9.87761685254435	9.29932103284875
O	6.93247682987641	9.90430039068760	9.27178687986851
H	5.67256072784916	13.10332050089105	8.76977177427879
H	4.09516511651159	10.22075971067688	10.16175679525809
H	5.87760266576849	9.85874315045232	9.29502836668427
H	7.27212035127695	9.01145545316988	9.44227929108781
O	4.44987485141948	15.26094997541199	9.20720320280765
O	6.95359866451158	15.28199527842398	9.24698947548152
H	4.14009269764028	15.52960163032700	10.08604446790753
H	5.86929270289399	15.23840810893770	9.25498461832170
H	7.32237510729372	14.38549196947562	9.24389876698212

10) Bare cluster + 2H₂O-OH*

Energy=-8570.719060271775

H	5.77741509660635	18.48719917280744	2.80454892013952
H	5.77741497275328	13.04046342963501	2.76833018434987
H	5.77741494927367	7.59242009490570	2.73413665664967
H	13.48063510287751	13.03905260135186	2.77042343832666
H	6.55859732777894	3.22350850390853	5.83627542515061
Ga	5.79874818749629	19.10892104520017	5.97392934377666
Ga	5.74087669706296	13.74093341222618	5.94769516693517
Ga	5.72612786832848	8.27822128658521	5.98141025992090
Ga	13.44873419151342	13.70096268128034	6.03508340660294
H	12.70392630107721	8.66726175433714	5.87242506478024
H	1.92580497780557	13.03905185513938	2.77042455965891
H	9.62902511170071	18.48719933248399	2.80454885539747
H	9.62902506465048	13.04046308094474	2.76833078732381
H	9.62902483369278	7.59242105136500	2.73413536441404
H	0.77682472442434	11.44172600220775	3.92960755364243
H	14.62961386998431	11.44172602244268	3.92960799937098
Ga	7.70464621288146	16.34917453658526	3.89244889808718
Ga	7.68317620684318	10.93621713922039	3.84330602710571
Ga	7.69283340882098	5.42972803151827	3.84087614600179
Ga	7.70858893775036	21.83693943664830	3.89573366908691
Ga	3.82616303591658	16.33985617726593	3.90991591402912
Ga	3.82331938212828	10.88761517962896	3.87515327854684
H	4.62962023833539	5.99564054144484	3.89357730295223
Ga	11.56447670603951	16.35363436283528	3.88880142317245
Ga	11.55217002340014	10.90048275726526	3.85396468353782
H	10.77682055941844	5.99563918014540	3.89357707821837
Ga	1.98781174419037	13.71701233996198	6.09921331490609
H	2.70251342576326	8.66726131366713	5.87242543169023
H	8.84784138921840	3.22350891340455	5.83627573503923
Ga	9.59450040004865	19.09574706623191	6.03720031268225
Ga	9.55694307642027	13.68082738026051	6.04128170751609
Ga	9.62397754524773	8.25673858519252	5.97349924595194
H	0.74840064733582	11.67346250201831	7.64098897509100

H	14.65803972403380	11.67346262666646	7.64098961897070
Ga	7.57508297462217	16.57509977193704	7.74073264390869
Ga	7.57781166408229	11.10507428676633	7.65694384889688
Ga	7.69880886864648	5.76728822437802	7.52769107611739
Ga	7.70279463054122	22.18086505007502	7.42900260495267
Ga	3.95449068427006	16.61964863305030	7.79876875628025
Ga	3.82488641340989	11.07812815709311	7.85263371955318
H	4.60139091037003	6.22734727033303	7.60533348128725
Ga	11.48135006358085	16.72034476017271	7.51668823867699
Ga	11.61582204431928	11.23775136522638	7.57464018605895
H	10.80504968239946	6.22734636450792	7.60533302002984
P	5.78218167513488	17.71756529093862	3.99779771168892
P	5.74772458137975	12.31127191387829	3.98465841993304
P	5.76213727667578	6.85985072261051	3.96345432926504
H	6.38704549487609	22.71684348544797	4.00420321217758
H	12.85194062126943	17.25642354350571	3.96807752356869
P	13.48038533631490	12.29072873325019	3.98936252612414
P	5.80780259299305	18.04826995034007	8.05002314867862
P	5.73097676033878	12.47954259515425	7.90345326226733
P	5.74248609120425	6.98745376258093	7.98850717020579
H	6.39778612260736	22.90385789679788	7.89512875063416
H	12.85064293753394	17.45114205398655	7.85597217188368
P	13.55221641830184	12.45486991718009	8.08818780447191
H	7.70321979574762	4.53002827919316	2.61196079905285
H	7.70322008440818	20.84237175105033	2.68056191956339
H	7.70322007176869	15.40326649295711	2.65531099267211
H	7.70321991951899	9.95986302541506	2.62421706726188
H	3.85161004925881	15.39798400493919	2.64793619547208
H	3.85160995962796	9.96381132044094	2.62972788296401
H	11.55483007562525	15.39798445323871	2.64793745808127
H	11.55482988983215	9.96381194973002	2.62972871116463
H	2.55450152084684	17.25642177144567	3.96807765633947
P	1.91847605604223	12.30694700379428	4.00321123904478
P	9.61835072057973	17.72694807002480	4.01064684606604
P	9.62974446277788	12.31239059012648	3.99701587118503
P	9.63621537514102	6.85065692489807	3.95656045963809
H	9.01939440782314	22.71684273014394	4.00420262826894
H	0.63926644705047	14.47657186759126	5.89317725950001
H	14.76717412323923	14.47657321186948	5.89317632880710
P	7.70436876267089	4.06383399063459	5.85114770574722
P	7.70806462837938	20.48014456863503	5.88333542952752
P	7.67800530680864	15.07822086860558	5.90225501166616
P	7.68719234270550	9.58849532187393	5.82220257835772
H	4.48384901681631	19.92840927015274	5.92900072358712
P	3.86767391359427	15.11577235328112	5.93081145380940
P	3.77730714195104	9.60587934524747	5.91123840220208
H	10.92259274974294	19.92841041516081	5.92900134624911
P	11.50428661438343	15.01000196649059	5.91177636811851
P	11.59987767560582	9.56275770957019	5.87985919588553

H	2.55579664488177	17.45114110195832	7.85597167651567
P	1.86933750934347	12.42997308098426	8.10137850493457
P	9.56125545180708	17.82286125673865	8.13671231264147
P	9.59859592158249	12.32420851781994	8.05270609714669
P	9.66667316341960	7.00139610842146	7.99448695835574
H	9.00865278059107	22.90385816811448	7.89512905945222
O	4.34780377833839	9.80075219952581	9.24333648764422
O	6.92729028337477	9.84813221497307	9.22956110938888
H	4.10836621229305	10.16306454419957	10.11153279284068
H	5.88324187725254	9.78761576089810	9.24622465018280
H	7.26742019542251	8.94336179811917	9.30653521203966
O	4.33166422403393	15.41643341013411	9.30994107537518
O	6.91175343696986	15.21415813262765	9.24487106664876
H	4.17758242869414	15.93250293874101	10.11797137299699
H	5.87040221460680	15.30407150864803	9.29160113763498
H	7.01123470416145	14.27135362198043	8.99791220958462

11) Co-adsorbed H_1^+* and $H_2^+* + 2H_2O-OH^+*$

Energy=-8571.667883270584

H	5.77741515783840	18.48719920665126	2.80454893342726
H	5.77741495982227	13.04046338931977	2.76833019105997
H	5.77741493674865	7.59242009704317	2.73413665361305
H	13.48063511520935	13.03905260080642	2.77042343140629
H	6.55859734531375	3.22350849117246	5.83627543198782
Ga	5.79408100636406	19.09732430673112	5.98730640180522
Ga	5.75708667914433	13.80393272270796	5.80876632452709
Ga	5.72967639551328	8.25150543132793	5.98442110357937
Ga	13.47280932454250	13.66988355754683	6.02144948435590
H	12.70392627534085	8.66726175637238	5.87242509726740
H	1.92580497580583	13.03905187241878	2.77042454023062
H	9.62902509738741	18.48719929790479	2.80454878011908
H	9.62902504293731	13.04046309387052	2.76833077657687
H	9.62902483668594	7.59242105233017	2.73413535862140
H	0.77682472581214	11.44172598099484	3.92960757469593
H	14.62961387231224	11.44172599847959	3.92960799559434
Ga	7.69086719173447	16.36469790236707	3.87103977084467
Ga	7.70202351447782	10.93126781263528	3.83892172384757
Ga	7.69323746098156	5.41984720596266	3.84560628124088
Ga	7.70423412985908	21.84770274776967	3.88327015415582
Ga	3.81918822999660	16.35491265957612	3.88466784557721
Ga	3.79999355239730	10.88247251954331	3.86898919525755
H	4.62962024987571	5.99564053591632	3.89357731439943
Ga	11.58230966181508	16.35521919690617	3.86812789356878
Ga	11.56674764828727	10.89013025428810	3.85514225180875
H	10.77682055188570	5.99563918026604	3.89357708065381
Ga	1.97062574872269	13.69638818913672	6.08465461676669
H	2.70251343624135	8.66726132617679	5.87242543553117
H	8.84784135784864	3.22350893200213	5.83627573057684
Ga	9.58248633796577	19.14473093078761	5.89898356286588

Ga	9.55119499114324	13.65097333201376	6.02678805779190
Ga	9.63690656349560	8.23497898071451	5.96728420372516
H	0.74840064685028	11.67346249036233	7.64098897421476
H	14.65803975200565	11.67346258205969	7.64098960584827
Ga	7.42769226274901	16.39437204490849	7.86015084217513
Ga	7.70345769651311	11.01704245756321	7.70406247619870
Ga	7.69844542294158	5.76461260537524	7.53914537650661
Ga	7.70371231809594	22.19405234040600	7.43559524270680
Ga	3.93714124849887	16.66652316859778	7.72021193048975
Ga	3.68473719333438	10.97805180532584	7.87216603134209
H	4.60139092302545	6.22734726726003	7.60533347411295
Ga	11.58639403569072	16.63778672125718	7.47138815513833
Ga	11.63724994955832	11.22877091372214	7.59497974532090
H	10.80504967121338	6.22734635678333	7.60533301022520
P	5.77674027852671	17.72192869049667	3.99997709705666
P	5.74774087103416	12.28817930036720	3.96138709997313
P	5.76435300555566	6.85600756856044	3.96011289908454
H	6.38704553699325	22.71684346540743	4.00420320081527
H	12.85194065331593	17.25642352057084	3.96807749048190
P	13.48234266444734	12.28589471977820	3.98392219772101
P	5.80382819122583	18.01544136825379	8.08322962655174
P	5.70723398501371	12.28661134319784	7.61497535238329
P	5.73854312737623	6.99162155788128	8.00011159556745
H	6.39778642991053	22.90385779991031	7.89512871632880
H	12.85064295412312	17.45114199763085	7.85597202155897
P	13.56007980167377	12.46270421374775	8.09264019174984
H	7.70321980471073	4.53002828428551	2.61196080101711
H	7.70322007342518	20.84237179923834	2.68056195714082
H	7.70322005653778	15.40326647027658	2.65531098097223
H	7.70321993914099	9.95986303894501	2.62421707175368
H	3.85161002241629	15.39798399484681	2.64793618874665
H	3.85160996532667	9.96381133024285	2.62972786417118
H	11.55483006392581	15.39798447067898	2.64793749011657
H	11.55482988908429	9.96381194864764	2.62972870934834
H	2.55450151954475	17.25642177177348	3.96807765503511
P	1.91401158753535	12.30683868268058	4.00026504858628
P	9.62116811476341	17.70701691146980	3.98487545245972
P	9.63860777975854	12.30379434599137	3.99080255828502
P	9.63437093720650	6.84611762671756	3.95222081884297
H	9.01939438167456	22.71684268575591	4.00420259614107
H	0.63926647453567	14.47657188030210	5.89317726638731
H	14.76717409188310	14.47657328110532	5.89317636659031
P	7.70397049301784	4.06354154823983	5.85784888263750
P	7.68718895303105	20.48637587065256	5.89140312491038
P	7.70043401418327	15.09118996261470	5.89095727077638
P	7.69221726711519	9.57870797159840	5.82367366844906
H	4.48384893666071	19.92840924573159	5.92900074295313
P	3.85280898304849	15.10973349611588	5.91243456912803
P	3.77959436917959	9.59149002033955	5.90771519227746

H	10.92259277914898	19.92841060566656	5.92900167011205
P	11.51148283344509	14.96892326138482	5.87445235982648
P	11.59938296712901	9.56422791451568	5.88685878658367
H	2.55579663265424	17.45114115489041	7.85597167953923
P	1.85090100535796	12.44526244516765	8.11332490629562
P	9.52369012910326	17.62207634592425	7.84185976180767
P	9.61586174254424	12.35108840845853	8.08129092446846
P	9.66765029462619	7.00286300769464	7.99646164591240
H	9.00865248739315	22.90385815275886	7.89512895632685
O	4.38235388452778	9.87662482576317	9.30532741866759
O	6.93574985697527	9.90227891881268	9.27453759831586
H	5.73138001868528	13.09969991867813	8.76028623142434
H	4.09793203215665	10.21666902055282	10.16853781468618
H	5.88111878360273	9.85549792305542	9.30016037398476
H	7.27998548815142	9.01325715839236	9.45554646345804
O	4.36204914581438	15.23438206122839	9.24781863453293
O	7.02310030513198	15.15172990733658	9.27724967024864
H	4.02297942649026	15.46221211117832	10.12737543521673
H	5.36668830953936	15.14781356965304	9.33544266237742
H	7.48495682010777	14.30338979067512	9.19961289523920
H	9.69074265638983	18.50076582493332	8.93042012932677

12) Adsorbed $\text{H}_2^+ + 2\text{H}_2\text{O}-\text{OH}^*$

Energy=-8571.197169345633

H	5.77741507847686	18.48719915055506	2.80454890671051
H	5.77741495865193	13.04046335720969	2.76833023688911
H	5.77741493707362	7.59242009938855	2.73413665000120
H	13.48063509912377	13.03905258835780	2.77042345288066
H	6.55859733738734	3.22350849220475	5.83627542986228
Ga	5.79762682535066	19.10037663339150	5.97589713261094
Ga	5.74820792713228	13.71343174540382	5.93916591811381
Ga	5.72799605808885	8.27482821103807	5.98126436808045
Ga	13.46811586930782	13.67195225211990	6.02176978675551
H	12.70392629174927	8.66726175762451	5.87242506391016
H	1.92580498045026	13.03905184999971	2.77042457003374
H	9.62902511752469	18.48719938243873	2.80454884005977
H	9.62902504880183	13.04046304704334	2.76833078483430
H	9.62902484111555	7.59242104715375	2.73413536237755
H	0.77682472886766	11.44172600190618	3.92960755303672
H	14.62961388733734	11.44172603592956	3.92960798023861
Ga	7.68026661949328	16.34267913965145	3.89343184738012
Ga	7.68177854936628	10.92809946107039	3.84714238323039
Ga	7.69312646180116	5.42829430705394	3.84134772093326
Ga	7.70549926562691	21.84627574301301	3.88510975705342
Ga	3.81981357689572	16.34156697037936	3.89988029354351
Ga	3.81808203093690	10.88058412360441	3.87661164571060
H	4.62962024615941	5.99564052814881	3.89357731097682
Ga	11.57808352955766	16.35427693196033	3.87166230339800
Ga	11.55090681684331	10.89371440290549	3.85679500030573

H	10.77682054970774	5.99563918698127	3.89357707990327
Ga	1.97496609818414	13.70178449839827	6.09709801364446
H	2.70251348090928	8.66726135119938	5.87242544175277
H	8.84784137706607	3.22350892795844	5.83627572861399
Ga	9.58384452887666	19.13310036427659	5.90156933412927
Ga	9.54057422817287	13.65558772254584	6.04449046415407
Ga	9.62031040444063	8.25423827882109	5.97540835331047
H	0.74840066530596	11.67346250532414	7.64098897132563
H	14.65803973372700	11.67346263267338	7.64098961925991
Ga	7.40253932060461	16.38196623367348	7.87096829037979
Ga	7.56938578185538	11.10891710295751	7.67534932907443
Ga	7.69827139147671	5.76480603092253	7.52953473615435
Ga	7.70370447677732	22.19144069177408	7.43266440767606
Ga	3.93309087289416	16.67235444820265	7.69364865314777
Ga	3.82698185080573	11.07380505261732	7.84909088554982
H	4.60139090381737	6.22734726106575	7.60533347471847
Ga	11.58286674393959	16.63913152299962	7.46682206297587
Ga	11.61530214337609	11.23245837926891	7.57712787101222
H	10.80504967358519	6.22734636521907	7.60533302506315
P	5.77516563305068	17.71906584479364	3.99793433098694
P	5.74517890623685	12.30229921593991	3.97830910734770
P	5.76290261398064	6.85909684620276	3.96284620608990
H	6.38704548013042	22.71684348311843	4.00420321481301
H	12.85194064217418	17.25642356226464	3.96807753385619
P	13.47856436710405	12.28332305170906	3.98322668806961
P	5.79734561745146	18.03221218843373	8.06722137565858
P	5.72148991642007	12.48943148870967	7.91215105916197
P	5.74260305920550	6.98695646631543	7.98935828758252
H	6.39778624791710	22.90385786501243	7.89512871494653
H	12.85064299634635	17.45114199056970	7.85597214687374
P	13.55078511426320	12.45448104432073	8.08575361080798
H	7.70321979714070	4.53002828296004	2.61196079912845
H	7.70322008918390	20.84237174494083	2.68056191306521
H	7.70322011383258	15.40326645290754	2.65531097714642
H	7.70321993908425	9.95986305743187	2.62421703743326
H	3.85161005093553	15.39798403154266	2.64793620679521
H	3.85160994310865	9.96381133252706	2.62972785749262
H	11.55483005685671	15.39798439756010	2.64793744074278
H	11.55482989451110	9.96381196882396	2.62972872048156
H	2.55450152934739	17.25642176144257	3.96807765891699
P	1.91877355240252	12.30475720737539	4.00115771199306
P	9.61296293359069	17.70082208860133	3.98337206218128
P	9.62714729315056	12.30776857965424	3.99425979367924
P	9.63564048704894	6.85055506059150	3.95646360028500
H	9.01939441454210	22.71684272289358	4.00420262617811
H	0.63926641452562	14.47657189237209	5.89317724150210
H	14.76717406997746	14.47657316972569	5.89317634326705
P	7.70433615889964	4.06360870209753	5.85166219001150
P	7.69259151816240	20.48641142993500	5.88710361065673

P	7.67464804469202	15.07642415437680	5.90693742376820
P	7.68543522178654	9.59433036815219	5.83257910338004
H	4.48384898511228	19.92840933341923	5.92900073343697
P	3.86875055382988	15.09495077507570	5.91656158154390
P	3.77915772201510	9.60271002882159	5.91117584644416
H	10.92259270415889	19.92841057261300	5.92900143337696
P	11.50892013637290	14.97047545761209	5.87271425729460
P	11.59767771290130	9.55999637511657	5.88209691393798
H	2.55579664734679	17.45114107922686	7.85597169380717
P	1.87123683087036	12.42589276897876	8.10173645618340
P	9.51639259948948	17.61507718606549	7.84641910202103
P	9.59847417721086	12.32449972879044	8.06110161455392
P	9.66596261362476	6.99997005166291	7.99589070855728
H	9.00865266949589	22.90385813712209	7.89512903999008
O	4.35210605261140	9.80095393120820	9.24434326635845
O	6.92141630189161	9.85342575848009	9.23684471927963
H	4.09936529182457	10.15519688026777	10.11205846935919
H	5.87404863711654	9.79031907145534	9.25492361164878
H	7.26430840937798	8.94982452003087	9.31620710732981
O	4.30838153340034	15.36963120988721	9.33442858475238
O	7.00897718274757	15.21332133142742	9.35158542743018
H	4.05480665127947	15.78410327076950	10.17498286697773
H	5.31189180326546	15.24516717585612	9.38446690597460
H	7.12129141493818	14.27595707760334	9.11397708248040
H	9.70280526246898	18.50781425151753	8.92134263358117

13) Adsorbed $H_1^+ + 2H_2O-OH^* + 3H_2O^*$

Energy=-8800.478446300258	H	5.77741512946523	18.48719920334192	2.80454892802419
H	5.77741493771896	13.04046341748800	2.76833020940921	
H	5.77741493582684	7.59242009080566	2.73413664926354	
H	13.48063509614932	13.03905259513365	2.77042343987939	
H	6.55859737068989	3.22350849600713	5.83627543511794	
Ga	5.82195892378414	19.14323312227681	5.95469463912361	
Ga	5.75875047751927	13.85161504991147	5.81653109985324	
Ga	5.73799667437690	8.27090268539008	5.98575683323883	
Ga	13.43595300181289	13.69759652912622	6.03672212356016	
H	12.70392629006523	8.66726174870932	5.87242507923351	
H	1.92580495603947	13.03905183921299	2.77042456841676	
H	9.62902520508861	18.48719931618661	2.80454880375853	
H	9.62902505213948	13.04046307091293	2.76833079271069	
H	9.62902483716757	7.59242104534154	2.73413536668939	
H	0.77682475021011	11.44172601980651	3.92960754908917	
H	14.62961388699484	11.44172602638451	3.92960798678121	
Ga	7.71891162333673	16.37093203113892	3.87589577302775	
Ga	7.70552025670846	10.94173864265487	3.83925033920796	
Ga	7.69153562654074	5.42244522275834	3.84461349749277	
Ga	7.70808524615561	21.82427664445399	3.91637203867775	
Ga	3.82948373491265	16.36093367572789	3.88994750634845	
Ga	3.81016071710702	10.89388259085808	3.86634099158841	

H	4.62962025349697	5.99564054025928	3.89357731034717
Ga	11.56905419637403	16.35112172569976	3.89104247287649
Ga	11.57196765231514	10.89872589825580	3.85651710392135
H	10.77682055698953	5.99563918287274	3.89357707702485
Ga	1.98649128003947	13.71714739176976	6.08669365553230
H	2.70251343863900	8.66726133426755	5.87242543634921
H	8.84784134010362	3.22350893195217	5.83627573130795
Ga	9.59797717843332	19.08830243556881	6.03990432576223
Ga	9.58981506097433	13.69506338488623	6.00903753733804
Ga	9.65690326535687	8.26477369758920	5.94220918518140
H	0.74840065151308	11.67346249523235	7.64098896832396
H	14.65803972140373	11.67346263523218	7.64098961178853
Ga	7.60366797526134	16.62519239149813	7.74803965846104
Ga	7.70495637764936	11.07436819760535	7.71928173791864
Ga	7.69087320096222	5.77667190195518	7.54368062385561
Ga	7.70417543810994	22.03355663684580	7.64276468344303
Ga	3.96313763736714	16.62402647173247	7.82255706745486
Ga	3.68835641271886	10.99420294135379	7.86360394823334
H	4.60139091691730	6.22734726714756	7.60533347605673
Ga	11.51104098103212	16.60294180827303	7.68373991835989
Ga	11.60281940146291	11.12566349066790	7.74544431796689
H	10.80504966937009	6.22734636278315	7.60533301483139
P	5.78646655989396	17.72198736217528	3.99807505959451
P	5.75316392890630	12.30487296272956	3.97293539130773
P	5.76370603135206	6.85997952311086	3.96284020622569
H	6.38704549429970	22.71684348158485	4.00420321751759
H	12.85194059544033	17.25642353383720	3.96807752977816
P	13.48512601470533	12.29546424490870	3.99028564607164
P	5.80829311007192	18.06373658784559	8.04074915362942
P	5.69538908550851	12.31528980392421	7.61358205016442
P	5.73366944517259	7.00053786961778	8.00076639568458
H	6.39778624299326	22.90385787254886	7.89512873230490
H	12.85064299618835	17.45114200890303	7.85597216908941
P	13.53529017870911	12.44169741234886	8.07353705298446
H	7.70321979990249	4.53002828055966	2.61196078974130
H	7.70322007613260	20.84237175151169	2.68056192039909
H	7.70322004563375	15.40326649080262	2.65531097571647
H	7.70321993294971	9.95986304882621	2.62421707586976
H	3.85161004107265	15.39798402902952	2.64793623816795
H	3.85160997941188	9.96381132570328	2.62972788968780
H	11.55483006430310	15.39798443422358	2.64793744939046
H	11.55482989324315	9.96381196084919	2.62972870940959
H	2.55450151459281	17.25642176046385	3.96807761840359
P	1.91440381484574	12.30960084030064	4.00263080828165
P	9.63129449918924	17.73034904029024	4.00928692597813
P	9.64194868274987	12.31072710691022	3.99343709118424
P	9.63350688487806	6.84688876661651	3.95136568649002
H	9.01939443241809	22.71684272484559	4.00420261732917
H	0.63926640146676	14.47657189399024	5.89317725944620

H	14.76717409237738	14.47657318761346	5.89317634374049
P	7.70511187569435	4.06676530897424	5.86025006841062
P	7.72590337282746	20.50017197938940	5.88342848701352
P	7.71248646194485	15.11356783844257	5.90428147251189
P	7.70038045210139	9.60477925136622	5.84222275129815
H	4.48384900589519	19.92840927237843	5.92900072120730
P	3.85273446008266	15.14304976100114	5.92432868734797
P	3.77783698700441	9.59526410164066	5.90563363699973
H	10.92259256157590	19.92841054818793	5.92900143593212
P	11.51308102133620	15.04016704082214	5.90048613653458
P	11.61461887487308	9.59027160490375	5.88627150613456
H	2.55579679469749	17.45114103872225	7.85597165679632
P	1.84845736139687	12.45081160094124	8.11111252864839
P	9.58418919871589	17.83882103893039	8.13369749594241
P	9.62487764340268	12.40254763197292	8.05313066245090
P	9.67424011086676	7.01629693057552	7.97223198203790
H	9.00865266198256	22.90385814319700	7.89512903136801
O	4.39347178159172	9.90335298805584	9.30683717273643
O	6.94051447783615	9.92579511736982	9.28088293534880
H	5.64955831568575	13.11916059756585	8.76663895714107
H	4.09769305167613	10.24114388040942	10.16711187577979
H	5.88134191747317	9.89510908638013	9.30672127805033
H	7.25340664414515	9.01681012913568	9.41228808398000
O	4.44825659481993	15.27568568205692	9.21028552683735
O	6.96685850117719	15.28334545951606	9.23840177767386
H	4.15512404945554	15.56150436767613	10.08957278233589
H	5.89367133815420	15.24666941270371	9.24938010518154
H	7.32065995714287	14.38133010672023	9.20174624330820
O	7.71301160382398	20.53807059388983	9.23091933943887
H	8.50113391959262	19.96008340814554	9.12715366237351
H	6.96828133614213	19.90764334827930	9.05854521537313
O	11.65004362668494	15.10977538930742	9.28395870309070
H	10.93055258885098	14.44917748455847	9.21912000890029
H	12.47056149691580	14.58026154057591	9.24914037267878
O	11.32344490160228	9.74325701112381	9.35360215203224
H	10.83750793695560	8.92033379902725	9.13161495549787
H	12.13011708447910	9.46011066511247	9.81579948019167

14) Bare cluster + 2H₂O-OH⁻* +3H₂O*

Energy=-8800.004919312762	H	5.77741513446778	18.48719921080785	2.80454892746868
H	5.77741493020990	13.04046341760651	2.76833020655248	
H	5.77741493919265	7.59242009314654	2.73413665450148	
H	13.48063508641790	13.03905259841505	2.77042344099712	
H	6.55859737297828	3.22350849731554	5.83627543015415	
Ga	5.82623240386113	19.14187118983920	5.95093605137734	
Ga	5.75333444693519	13.75812636127815	5.94884853656359	
Ga	5.73395801172981	8.29317780831199	5.98412982686917	
Ga	13.43262669767591	13.69809378984228	6.03531316119705	
H	12.70392629220083	8.66726174793809	5.87242507278613	

H	1.92580494004679	13.03905184403375	2.77042456048723
H	9.62902519998264	18.48719932356404	2.80454879925308
H	9.62902505879788	13.04046307370137	2.76833079551290
H	9.62902484038326	7.59242104258527	2.73413537231078
H	0.77682476427394	11.44172602151761	3.92960755846709
H	14.62961389162862	11.44172602057843	3.92960798833293
Ga	7.70821353917626	16.35204516500815	3.89373795373072
Ga	7.68497922225970	10.93896151106989	3.84552873012856
Ga	7.68774961175760	5.42992535165028	3.84049340625163
Ga	7.70866776451814	21.82318533353829	3.91718389317776
Ga	3.83078526427402	16.34569160205370	3.90834867675135
Ga	3.82614468681417	10.89142182640704	3.87430133181982
H	4.62962025022660	5.99564054031687	3.89357731047427
Ga	11.56586060381902	16.35063156463627	3.89374045534762
Ga	11.55732381407909	10.90376537722884	3.85477640544029
H	10.77682055810850	5.99563918276616	3.89357707492672
Ga	1.99184582589654	13.72342810974087	6.10211534471101
H	2.70251342604764	8.66726132841516	5.87242544493927
H	8.84784133558709	3.22350893326700	5.83627572908054
Ga	9.59814874273602	19.07853836592876	6.04100787739190
Ga	9.58468406205963	13.69331695560094	6.02230717051212
Ga	9.64207268727989	8.27549710604680	5.94184935534270
H	0.74840062642442	11.67346247558102	7.64098896765027
H	14.65803973304172	11.67346262938967	7.64098961333023
Ga	7.59363390183747	16.59569849491098	7.74501044118555
Ga	7.58650910877154	11.14850078526044	7.67440131592429
Ga	7.68784400119350	5.77631267865889	7.53412770480838
Ga	7.70425584778822	22.03070854735921	7.63880477808916
Ga	3.95668159102912	16.63090682290610	7.80028526044390
Ga	3.82763128349980	11.08452678545569	7.85054121352396
H	4.60139091692393	6.22734727053247	7.60533347671660
Ga	11.50988126738514	16.59497486897534	7.68047071319500
Ga	11.58505687322509	11.12475777230562	7.72146702297407
H	10.80504967469385	6.22734636260285	7.60533301681910
P	5.78402486267944	17.72001104864600	3.99783932739718
P	5.74940380213315	12.31678662038569	3.98811783033920
P	5.76116597083812	6.86360573833534	3.96590429785980
H	6.38704549219700	22.71684348346007	4.00420321993503
H	12.85194059968830	17.25642353666261	3.96807752918424
P	13.48183929588937	12.29290580293395	3.98930112706090
P	5.81506491654323	18.06334444852286	8.03120861841018
P	5.72276950996844	12.49629683337974	7.90506854928690
P	5.73628481820691	6.99648580925106	7.99238718857931
H	6.39778623595746	22.90385787240988	7.89512873442510
H	12.85064299918633	17.45114200829467	7.85597217232914
P	13.52666236897634	12.43220707577832	8.06639432831562
H	7.70321979685026	4.53002828186800	2.61196079578696
H	7.70322007393342	20.84237174867675	2.68056191586284
H	7.70322004705350	15.40326649143562	2.65531097685424

H	7.70321993079900	9.95986303613758	2.62421706821440
H	3.85161005165599	15.39798401369911	2.64793623275761
H	3.85160998461296	9.96381132418689	2.62972788290627
H	11.55483006393222	15.39798443464092	2.64793744886374
H	11.55482989268720	9.96381196055155	2.62972871908695
H	2.55450148724992	17.25642177928130	3.96807762207925
P	1.91862294159234	12.30834817929315	4.00421579907394
P	9.62395921570148	17.72411672708426	4.00805806576342
P	9.63146201899323	12.31172644784851	3.99459833401767
P	9.63371419109973	6.84771171480507	3.95275624604159
H	9.01939443386866	22.71684272605808	4.00420261816198
H	0.63926642344436	14.47657190552396	5.89317725700418
H	14.76717409821589	14.47657319682714	5.89317634782501
P	7.70538497942530	4.06667958288473	5.85437688105851
P	7.72995595772969	20.50022079673300	5.87910063818742
P	7.69187058481969	15.08971886197360	5.90664962438169
P	7.69738342589206	9.60823322481750	5.84035920651092
H	4.48384901877192	19.92840926140198	5.92900072315826
P	3.87276815423989	15.12548637732935	5.93278963467243
P	3.77689861729760	9.60841884075857	5.91137582991438
H	10.92259257508683	19.92841055952676	5.92900143184872
P	11.51186850960771	15.03901201814591	5.89470388077503
P	11.61176461605425	9.58462093575250	5.87557924671977
H	2.55579677140100	17.45114105080810	7.85597166405908
P	1.86881626274159	12.43102878397943	8.10175192188705
P	9.57762743315407	17.82390050480618	8.13407293911713
P	9.61282388011450	12.37121943811832	8.03399891350865
P	9.67083137972122	7.01320279433008	7.96926364300668
H	9.00865266904781	22.90385814249111	7.89512903047027
O	4.35918331211739	9.81291558411177	9.24593354571447
O	6.93733537997965	9.86730449465703	9.23587327131401
H	4.11281846852060	10.17316035081010	10.11304817734876
H	5.89104987250674	9.81294210194402	9.25257196535756
H	7.26158727853516	8.95536703308334	9.29250186399858
O	4.34238217325526	15.43494195653072	9.31176190800482
O	6.92676336296094	15.23271211543467	9.24732410539263
H	4.19974591408741	15.95767718810294	10.11763406196188
H	5.88587571050843	15.31273880048957	9.28788331495956
H	7.04507639138905	14.29116227500325	9.00828066565169
O	7.71191421299772	20.52613178220004	9.21819066374958
H	8.50190359124028	19.95049686332533	9.11200275454044
H	6.97009317989030	19.89299254251245	9.03360130958644
O	11.61740610842207	15.06600544795260	9.25839977385747
H	10.91336538435941	14.39449902217779	9.12647863306102
H	12.44751664990775	14.55076743164331	9.23304972125424
O	11.35628768846960	9.70779772008104	9.32482834701016
H	10.79952686172975	8.92319629466131	9.13233337447627
H	12.17354092621246	9.36821072488046	9.72495291399363

15) Co-adsorbed H_1^+* and $H_2^+* + 2H_2O-OH^* + 3H_2O^*$

Energy=-8801.007803842922

H	5.77741508807347	18.48719919878191	2.80454894254909
H	5.77741494079666	13.04046338828838	2.76833019867889
H	5.77741493145635	7.59242008685126	2.73413663932513
H	13.48063509568830	13.03905259370702	2.77042344282761
H	6.55859741771830	3.22350854937197	5.83627545012118
Ga	5.84078323874342	19.21346531114569	5.81036176591710
Ga	5.75820657380413	13.81130700035595	5.81736354222927
Ga	5.73958174562838	8.26502664560160	5.98503328066382
Ga	13.44021088309833	13.69444016026699	6.03988699636876
H	12.70392631299848	8.66726174032256	5.87242507592473
H	1.92580497612067	13.03905184677864	2.77042456245172
H	9.62902518668188	18.48719932586580	2.80454880477686
H	9.62902505576630	13.04046306464681	2.76833078771547
H	9.62902482418361	7.59242103361114	2.73413539246762
H	0.77682472771636	11.44172600271799	3.92960755012610
H	14.62961388356352	11.44172602872067	3.92960798748998
Ga	7.73953513787404	16.36735158445826	3.87123582247413
Ga	7.71007268057876	10.93324011768288	3.84181536847132
Ga	7.69214928939395	5.42041913060255	3.84546305722736
Ga	7.71131154646104	21.83717699389176	3.90296143813509
Ga	3.81439996306527	16.35610424201684	3.88292965947051
Ga	3.80973580866476	10.88342567628362	3.86938285715438
H	4.62962023520960	5.99564053090883	3.89357731139811
Ga	11.58020922472130	16.34470857224522	3.89053097896596
Ga	11.58395466413551	10.89112738358699	3.85736315523624
H	10.77682056483826	5.99563917768110	3.89357707276472
Ga	1.96290525179661	13.67895745605460	6.06701535030263
H	2.70251349412914	8.66726136809630	5.87242540918502
H	8.84784132250002	3.22350893037044	5.83627573128480
Ga	9.60872359380801	19.07395017838155	6.03124458492827
Ga	9.61601776331999	13.65494329796357	5.99616795073430
Ga	9.65862717085267	8.26098713185299	5.94213806706495
H	0.74840065587027	11.67346249507667	7.64098897626303
H	14.65803972398813	11.67346263301038	7.64098961257124
Ga	7.73572837815731	16.48040478255057	7.75342549743622
Ga	7.71140046243404	11.06854327765307	7.72657122089036
Ga	7.69126228884204	5.77482552800379	7.54516016154504
Ga	7.71081996256521	22.05520331099801	7.64497977482323
Ga	3.83822718977356	16.48845912318130	7.81735522117698
Ga	3.68724017177452	10.98581191817255	7.87166905888203
H	4.60139082812022	6.22734720619154	7.60533347951372
Ga	11.52780070794023	16.58744909271750	7.70050293487462
Ga	11.61053528174281	11.11865657473059	7.75249770664777
H	10.80504968645083	6.22734637168201	7.60533299599897
P	5.78976840918244	17.70125981959195	3.97530665420371
P	5.75476291378795	12.29276767458619	3.96542919633681
P	5.76450248543533	6.85875323384037	3.96182163925666

H	6.38704550568800	22.71684348288891	4.00420321453743
H	12.85194059696216	17.25642353344834	3.96807753518376
P	13.48688949887578	12.29681129158474	3.99085427615753
P	5.81000035918182	17.80642570871499	7.71164871801025
P	5.69959904374515	12.30916336444188	7.63038138330840
P	5.73398050929039	6.99950629592722	8.00178322079896
H	6.39778625795199	22.90385786235564	7.89512872367111
H	12.85064303825594	17.45114201345030	7.85597217681037
P	13.53733291050579	12.44171259181375	8.07676158482569
H	7.70321980306112	4.53002828342442	2.61196078746471
H	7.70322007448654	20.84237176142717	2.68056192884986
H	7.70322005328597	15.40326648767059	2.65531097773368
H	7.70321993624250	9.95986303718074	2.62421703764660
H	3.85161006026261	15.39798400251770	2.64793622094346
H	3.85160996975534	9.96381134646498	2.62972792259868
H	11.55483006747414	15.39798442653062	2.64793744423361
H	11.55482989091080	9.96381196109363	2.62972870851488
H	2.55450149785461	17.25642177690592	3.96807763034909
P	1.91650007751418	12.30026975179671	3.99517279272319
P	9.64081655585369	17.72674975024276	4.00671497250946
P	9.64987896772646	12.29592624973033	3.98351476402229
P	9.63337283247268	6.84636101985916	3.95084429905101
H	9.01939441555063	22.71684271541656	4.00420261656736
H	0.63926643849469	14.47657187849526	5.89317725709628
H	14.76717409138125	14.47657318973449	5.89317634448849
P	7.70518676254227	4.06637478162516	5.86122058891134
P	7.75193645991428	20.51073623322896	5.89122263384750
P	7.72606581161937	15.05961366565527	5.87749901781868
P	7.70139863161564	9.60364066764799	5.84611225904386
H	4.48384904994392	19.92840924061318	5.92900073121173
P	3.84011367523852	15.09460422210310	5.89551914248576
P	3.78019122376870	9.59239582347370	5.90885142446356
H	10.92259262213142	19.92841058946982	5.92900143028023
P	11.51223986776349	15.03977685032575	5.90419385414282
P	11.61523041607019	9.58964236924385	5.88875487076204
H	2.55579664848543	17.45114110271233	7.85597167348115
P	1.85027812544638	12.44860425940862	8.10833814492998
P	9.58791718304025	17.83325645105145	8.14894913410341
P	9.63168442370099	12.40014299591330	8.05520526919038
P	9.67441572082750	7.01580385958606	7.97319105372144
H	9.00865265251659	22.90385814237418	7.89512903060256
O	4.39781875608115	9.89774702326344	9.31178989030544
O	6.94621983978573	9.91954153744307	9.28400398202487
H	5.67087232337502	13.14006200600459	8.76447838884950
H	4.10021828758112	10.23006561762149	10.17356089580291
H	5.88704677873974	9.88936408044618	9.31159549202061
H	7.26038499973978	9.01147166614748	9.41898373752067
H	5.86688806159623	18.64074871014811	8.84817827390792
O	4.43482265100898	15.27736300617286	9.23387456029593

O	6.96438396017272	15.31175516421535	9.30677957715776
H	4.06725481626244	15.49490282099215	10.10379390516818
H	5.89926394125233	15.27459199195818	9.30924987613351
H	7.31921443239581	14.41954148471190	9.44290542100828
O	7.91858935859079	20.65688145062335	9.28600488896946
H	8.49024607482394	19.88665767664071	9.06313138131280
H	7.07886369828431	20.27659582273851	9.58935458366765
O	11.65249783530162	15.09798258138972	9.28657307463365
H	10.94510426982009	14.42435784049322	9.21589002920111
H	12.48268796252797	14.58232383762887	9.27256706316856
O	11.32579220618617	9.73940509208181	9.35645155321210
H	10.84034942109127	8.91641139573739	9.13344799727063
H	12.12989332961711	9.45689431479521	9.82369459445069

16) Adsorbed $\text{H}_2^+ + 2\text{H}_2\text{O}-\text{OH}^+ + 3\text{H}_2\text{O}^+$

Energy=-8800.482340246766

H	5.77741509791299	18.48719919307547	2.80454894939821
H	5.77741490897439	13.04046335168295	2.76833025144831
H	5.77741493643320	7.59242008709227	2.73413665970040
H	13.48063509743618	13.03905259671844	2.77042344289106
H	6.55859738489539	3.22350849763754	5.83627543283987
Ga	5.84289531923882	19.21168496370362	5.80791076659987
Ga	5.75494325627987	13.71845527216155	5.94523940709948
Ga	5.73476608286799	8.28834455308876	5.98426406473657
Ga	13.43662816909505	13.69546884723678	6.03860344105569
H	12.70392627593458	8.66726174855544	5.87242508046438
H	1.92580497799551	13.03905186019232	2.77042453470042
H	9.62902517464694	18.48719931508796	2.80454880035298
H	9.62902505715634	13.04046305237388	2.76833078226546
H	9.62902484092471	7.59242104348384	2.73413536552422
H	0.77682471093626	11.44172598567119	3.92960756427016
H	14.62961388353222	11.44172602850091	3.92960798540277
Ga	7.72962212848653	16.34944057301018	3.88802661042399
Ga	7.68926037917901	10.93024718368368	3.84814853246746
Ga	7.68847683991968	5.42823664356951	3.84123748982426
Ga	7.71180577933615	21.83557377567764	3.90470617864955
Ga	3.81431958282163	16.33825875235095	3.90727884533429
Ga	3.82552068895724	10.88006921863808	3.87803039691221
H	4.62962025707598	5.99564054332099	3.89357730834930
Ga	11.57715451465594	16.34420332923128	3.89327327452373
Ga	11.56956146091473	10.89653742553806	3.85537965839967
H	10.77682054745059	5.99563919061470	3.89357707694813
Ga	1.96792901840995	13.68433314765340	6.08193279728499
H	2.70251345587979	8.66726137477739	5.87242544006960
H	8.84784132772053	3.22350893008341	5.83627572886830
Ga	9.60909559822151	19.06460113616471	6.03181085513713
Ga	9.60974214081766	13.65466308840875	6.00501415111183
Ga	9.64339559283706	8.27304497896674	5.94233622035940
H	0.74840068944034	11.67346249404287	7.64098896808199

H	14.65803970151960	11.67346264633485	7.64098961248030
Ga	7.72563668946551	16.45637554290508	7.75033089381296
Ga	7.59182501108295	11.14429355488052	7.68490959419580
Ga	7.68836505447019	5.77490788563486	7.53537328766914
Ga	7.71140136800907	22.05307597129936	7.64034898362223
Ga	3.83688447963373	16.49613215217390	7.81657152727579
Ga	3.82572352709881	11.08138718373323	7.86292989873339
H	4.60139090770683	6.22734726026931	7.60533347695254
Ga	11.52568565363012	16.58063356059854	7.69668197529047
Ga	11.59288377920271	11.11844900641939	7.72879147137008
H	10.80504967628585	6.22734635855978	7.60533301688038
P	5.78684588683854	17.69915904125562	3.97524466669884
P	5.75043224283452	12.30444628903779	3.98036673382044
P	5.76162487563400	6.86285147716335	3.96523268837758
H	6.38704550952568	22.71684347984362	4.00420321379634
H	12.85194059165796	17.25642352996389	3.96807754570998
P	13.48373515698895	12.29447040750178	3.98997467687347
P	5.81687501450102	17.81100660688909	7.70429392530931
P	5.72707097588323	12.49749945615521	7.91931891869878
P	5.73656872787292	6.99586264485990	7.99343871266587
H	6.39778625663884	22.90385785933447	7.89512872284317
H	12.85064302888444	17.45114201437116	7.85597217791164
P	13.52883169089261	12.43271027324779	8.06985914464551
H	7.70321979850107	4.53002828920870	2.61196079714972
H	7.70322007540475	20.84237176627976	2.68056193252632
H	7.70322005402433	15.40326649799602	2.65531099373957
H	7.70321994804739	9.95986304729705	2.62421702522348
H	3.85161007207864	15.39798397933549	2.64793619735459
H	3.85160998367520	9.96381131944760	2.62972784341278
H	11.55483007145002	15.39798442348441	2.64793743554793
H	11.55482989752767	9.96381196128343	2.62972870959455
H	2.55450148042094	17.25642179526951	3.96807764470003
P	1.92089137796032	12.29906554443784	3.99679881357050
P	9.63366022349704	17.72087747564856	4.00527715552120
P	9.63923506898754	12.29638057368119	3.98404793142573
P	9.63361575724555	6.84760657923932	3.95249576803583
H	9.01939440948547	22.71684270989796	4.00420261631090
H	0.63926645443992	14.47657189239162	5.89317727107927
H	14.76717408622506	14.47657317322300	5.89317633970647
P	7.70541598198002	4.06637172522984	5.85509907189513
P	7.75484049993943	20.51005064846913	5.88778961798392
P	7.70604833423832	15.03901483382842	5.87745662051350
P	7.69743639425741	9.60869881984074	5.84573878692164
H	4.48384903483373	19.92840924562961	5.92900073298438
P	3.86106099743948	15.07665440878100	5.91813256011000
P	3.77831953501865	9.60728316392873	5.91803089286905
H	10.92259266819984	19.92841061678107	5.92900143103981
P	11.51102330806887	15.03890749750923	5.89812685870301
P	11.61247656426137	9.58423939724908	5.87829684916004

H	2.55579663792243	17.45114110614131	7.85597167848169
P	1.86806726809176	12.43139288212643	8.10062144987617
P	9.58115937471282	17.81981716065255	8.14835425052984
P	9.61980175391735	12.37008289350772	8.03303626626831
P	9.67112682970173	7.01336547884060	7.96992544917202
H	9.00865265376441	22.90385814160102	7.89512902869764
O	4.36515206960108	9.81470703003492	9.25567934145073
O	6.94068784297032	9.86650365390097	9.24128282234103
H	4.11501961713451	10.16934837816722	10.12403741139333
H	5.89367187294279	9.81320907328690	9.26124842860335
H	7.26554404859490	8.95496163605860	9.30196198035026
H	5.87777663913189	18.64693782233940	8.84002660558266
O	4.34970356716919	15.49497981196813	9.39986772677307
O	6.93708750030843	15.21444916720136	9.27215538743592
H	4.18903097220952	16.06198508124574	10.17123840660625
H	5.90921053519686	15.35582093139737	9.34708645973621
H	6.97848236835427	14.25873956199823	9.04817930599837
O	7.92631639358568	20.64884128063974	9.27816038869095
H	8.49617959450923	19.87891296093306	9.04659103000743
H	7.08607164857267	20.26538212349384	9.57632530055842
O	11.61184911333127	15.05603428871243	9.26008793015874
H	10.91255807131399	14.37884314726939	9.12700759060294
H	12.44541806848678	14.54552554042869	9.25214433133348
O	11.35493623725633	9.70827894242013	9.33073648698447
H	10.80094008620840	8.92162435721340	9.13849895086359
H	12.16918029848020	9.37314071661427	9.74080474047159

Surface charge effect on adsorbed proton acidity

Surface charge=-1

1) Bare cluster

Energy=-8265.93962429523

H	5.77741510719812	18.48719919963134	2.80454894719870
H	5.77741502187703	13.04046341187112	2.76833018797148
H	5.77741499349548	7.59242010712182	2.73413662412094
H	13.48063509793015	13.03905258760425	2.77042346985212
H	6.55859726761607	3.22350859358310	5.83627542540483
Ga	5.80420206380224	19.12636662335617	5.98487534456297
Ga	5.77194104362052	13.68181117174067	5.98956011953683
Ga	5.78115677429919	8.16746282142473	6.00355046077945
Ga	13.46375893866919	13.68817179175222	6.03735483165554
H	12.70392636101515	8.66726171830693	5.87242507275009
H	1.92580492742060	13.03905176329640	2.77042465562252
H	9.62902517411464	18.48719932880651	2.80454882226264
H	9.62902502955055	13.04046308825503	2.76833074243517
H	9.62902477993899	7.59242105527633	2.73413536143789
H	0.77682478758682	11.44172608391592	3.92960751089092
H	14.62961386311309	11.44172603904441	3.92960799291501
Ga	7.70326993850786	16.35493958480975	3.87304294414840
Ga	7.70328547684931	10.92224444742797	3.84196099166070

Ga	7.70281038903622	5.36254448319962	3.89849022937836
Ga	7.70320566226609	21.84462689791473	3.88603549296020
Ga	3.82873016424394	16.36050523848984	3.87067349633898
Ga	3.82983350927550	10.88521810449753	3.85674939881327
H	4.62962015974634	5.99564048179603	3.89357731343771
Ga	11.57773560760007	16.36037515449082	3.87083606060841
Ga	11.57672430651227	10.88514862517099	3.85678018968737
H	10.77682062759801	5.99563912553846	3.89357706268590
Ga	1.94303632605810	13.68860682023563	6.03700947749123
H	2.70251330494212	8.66726124049924	5.87242544167382
H	8.84784149715787	3.22350879930772	5.83627571323586
Ga	9.60221106237437	19.12633904172392	5.98486453939457
Ga	9.63451018537977	13.68179195129654	5.98963519272370
Ga	9.62525235681523	8.16747218472649	6.00348559706154
H	0.74840069532798	11.67346251290900	7.64098898474700
H	14.65803969932358	11.67346263927555	7.64098962419795
Ga	7.70323502873217	16.67209039878465	7.53488276024894
Ga	7.70307225758916	11.19691536887682	7.47351417416021
Ga	7.70307591869021	5.49496770931082	8.05683077661593
Ga	7.70323839359351	22.19219008116789	7.44572983891835
Ga	3.91266299543609	16.73821413381657	7.49515371398083
Ga	3.75969007970060	11.20191546319443	7.53975066143373
H	4.60139091990054	6.22734730115872	7.60533349702641
Ga	11.49399411966126	16.73787760598917	7.49495198213636
Ga	11.64682382243083	11.20185059316799	7.53990011033096
H	10.80504965083723	6.22734639809932	7.60533304041542
P	5.78541844193110	17.72242956179522	4.00482938943084
P	5.75977922006616	12.29994770184032	3.98489507669761
P	5.78178128128813	6.83362697935184	3.94912365376249
H	6.38704554542594	22.71684348073028	4.00420322540387
H	12.85194066190811	17.25642358930767	3.96807755851504
P	13.48432770939470	12.29220707772772	3.98846725769517
P	5.81524974183094	17.88701469984044	8.10702089376393
P	5.74739195770800	12.36841788828522	8.02169853864472
P	5.73259833876995	6.99916639157379	8.01898781707895
H	6.39778618183048	22.90385780828752	7.89512871572288
H	12.85064291498490	17.45114195834472	7.85597212262344
P	13.54891768024056	12.44702836945217	8.08862809345622
H	7.70321981597261	4.53002833040812	2.61196081163116
H	7.70322003825577	20.84237172982165	2.68056189804263
H	7.70322004254927	15.40326648992199	2.65531098913913
H	7.70321992563966	9.95986312374441	2.62421717617340
H	3.85161005859308	15.39798399889149	2.64793622406658
H	3.85160994587898	9.96381134248152	2.62972785510982
H	11.55483002066698	15.39798438727037	2.64793743272899
H	11.55482989560089	9.96381192951142	2.62972866328633
H	2.55450149315309	17.25642179069121	3.96807762672472
P	1.92213515206347	12.29218035170730	3.98842092683114
P	9.62108815104515	17.72242686320328	4.00482809618808

P	9.64674722811131	12.29993739541714	3.98492008028864
P	9.62447506006905	6.83339575336622	3.94900442173222
H	9.01939442193894	22.71684272204077	4.00420263409187
H	0.63926641145305	14.47657187473426	5.89317721051926
H	14.76717414434463	14.47657320806504	5.89317633859987
P	7.70319063726558	4.08704717556220	5.93636721273310
P	7.70322264104062	20.48263038373032	5.90259543950980
P	7.70323825991173	15.01913708085647	5.88823486195380
P	7.70320022721415	9.54662171951490	5.81297634853953
H	4.48384896299659	19.92840929005802	5.92900073199086
P	3.87093396077778	15.03368189621514	5.89509605626660
P	3.82237990310713	9.53797587510491	5.86312758416039
H	10.92259268201309	19.92841062384961	5.92900143094346
P	11.53576934225386	15.03330858116682	5.89523234799737
P	11.58406632085187	9.53794211641057	5.86303816768541
H	2.55579675630682	17.45114106177732	7.85597164792357
P	1.85757607616958	12.44720513756497	8.08821942328852
P	9.59134791994353	17.88676883557947	8.10688066263348
P	9.65893750068884	12.36802916865567	8.02180536688228
P	9.67370607121585	6.99902877113602	8.01886578567425
H	9.00865273736282	22.90385819162162	7.89512903747153

2) Adsorbed H₁⁺*

Energy=-8266.38476107945

H	5.77741508210488	18.48719920756210	2.80454893224581
H	5.77741503920222	13.04046336310308	2.76833020903604
H	5.77741507613331	7.59242021802461	2.73413661315921
H	13.48063512108772	13.03905254229962	2.77042350292078
H	6.55859751591444	3.22350853307214	5.83627545606664
Ga	5.80597897947234	19.13014115380141	5.98112807852236
Ga	5.79065276592422	13.69260845268174	5.90763795755575
Ga	5.80315434903729	8.25019231721507	5.98455296315249
Ga	13.46078357283110	13.69638662779622	6.04274832385097
H	12.70392622965450	8.66726181767915	5.87242504736689
H	1.92580492854519	13.03905172113991	2.77042470347990
H	9.62902520249636	18.48719934316143	2.80454881682125
H	9.62902504795256	13.04046304708825	2.76833076444363
H	9.62902485943438	7.59242108442170	2.73413532239294
H	0.77682479038257	11.44172611150151	3.92960748509155
H	14.62961384227484	11.44172607789927	3.92960796489699
Ga	7.71176733734491	16.35570279838639	3.87298580652398
Ga	7.72613269367034	10.91036202020439	3.85633352497568
Ga	7.70248675267048	5.41729162996394	3.85006225649846
Ga	7.70321509305440	21.84594189995020	3.88467158207102
Ga	3.82913320223619	16.36394680920768	3.86819505716703
Ga	3.82085936107223	10.89342842327593	3.84535615861369
H	4.62962005800574	5.99564038428107	3.89357732609969
Ga	11.58092994234341	16.35358281848688	3.87627551836544
Ga	11.58281613891726	10.88686521550870	3.85927610764652

H	10.77682060707506	5.99563916331963	3.89357710479841
Ga	1.94318480882237	13.69463757778176	6.02798831072292
H	2.70251342298214	8.66726131915292	5.87242540687132
H	8.84784121588203	3.22350896915964	5.83627574463146
Ga	9.60364607758178	19.12655090464752	5.98489030419322
Ga	9.62080183803132	13.62864799260312	6.01707183069517
Ga	9.62739826382836	8.25204776500152	5.96889368343644
H	0.74840069398478	11.67346251443669	7.64098898236593
H	14.65803977005412	11.67346261779259	7.64098962135882
Ga	7.70802599137301	16.67638184431916	7.53463303687973
Ga	7.90358650479249	10.78572626646802	8.04041131014874
Ga	7.70674545830919	5.78158866804814	7.56914954962187
Ga	7.70323237434289	22.19316585431404	7.44608407589557
Ga	3.91553002913783	16.74594754202244	7.49605695733818
Ga	3.64659417060924	11.17776932683243	7.57089979296959
H	4.60139090371357	6.22734727890799	7.60533348259470
Ga	11.49857177627216	16.72912686596081	7.48776703994577
Ga	11.66429114865192	11.24725850031969	7.59787821162104
H	10.80504973103489	6.22734634786814	7.60533302795628
P	5.78890944694125	17.72068808172601	4.00512368770332
P	5.76820905312144	12.27887841058966	3.96610213100234
P	5.76821242552079	6.85348629240034	3.95858053532703
H	6.38704546384592	22.71684358244639	4.00420332738338
H	12.85194062754351	17.25642356749303	3.96807753048987
P	13.48729620881155	12.29547830778934	3.99158578267218
P	5.81869499878724	17.88785778937052	8.10848841096339
P	5.79038879769734	12.15043458763816	7.78224451415558
P	5.72621591969461	7.00985712286520	8.01036147980741
H	6.39778605899430	22.90385780993581	7.89512872408912
H	12.85064299638832	17.45114198794710	7.85597214875501
P	13.58028411871979	12.46978846383971	8.10559365469524
H	7.70321975999352	4.53002819612973	2.61196072381382
H	7.70322016550619	20.84237165899731	2.68056186670550
H	7.70322004887347	15.40326647548739	2.65531098991453
H	7.70321989973187	9.95986311191510	2.62421715423424
H	3.85161003447497	15.39798404380788	2.64793625534626
H	3.85160993484576	9.96381133484410	2.62972784937538
H	11.55483003944806	15.39798440029176	2.64793744293882
H	11.55482991554194	9.96381193693144	2.62972871577679
H	2.55450154026822	17.25642174493952	3.96807759493206
P	1.91846403231499	12.29447499503889	3.98884692901229
P	9.62607559964160	17.72292119793308	4.00526672598202
P	9.65137403408518	12.29736246627042	3.98390364692108
P	9.63813844601676	6.85078371003295	3.95590275199239
H	9.01939440016011	22.71684269705014	4.00420258652375
H	0.63926638581968	14.47657186367570	5.89317721749952
H	14.76717409144675	14.47657318338032	5.89317634143655
P	7.70324055253019	4.06810478577199	5.87158661429606
P	7.70506658655462	20.48343357959623	5.90268745016605

P	7.71699374443430	15.01418536684638	5.89403668977604
P	7.71155603551885	9.63347796569746	5.86996524078156
H	4.48384898396153	19.92840927702172	5.92900072749681
P	3.87633835960836	15.02842609970219	5.90256110229776
P	3.80573810345954	9.55289374915286	5.86985521986000
H	10.92259257342467	19.92841056338989	5.92900141832588
P	11.51895001715660	15.01836938933350	5.89523365064438
P	11.60575695345718	9.56895179836084	5.89578414528882
H	2.55579672000102	17.45114108464456	7.85597166334050
P	1.81764494123727	12.48193851480067	8.11127328952029
P	9.59746204499117	17.88434321125469	8.10461297252610
P	9.69218170286568	12.40726473582702	8.07127676308390
P	9.68159122201773	7.01534924859045	8.00315415458753
H	9.00865286025621	22.90385821936411	7.89512903859830
H	5.60032673178375	13.04164419587725	8.85894714730340

3) Co-adsorbed H_1^+ and H_2^+

H	5.77741514944461	18.48719925091539	2.80454894475148
H	5.77741497982522	13.04046334716822	2.76833022415929
H	5.77741493766894	7.59242007511186	2.73413659523178
H	13.48063517716223	13.03905251201588	2.77042349972068
H	6.55859776021845	3.22350851439631	5.83627544422611
Ga	5.74870208968927	19.06774960942247	5.91375983932280
Ga	5.78390981328026	13.62953144788027	5.94290220933356
Ga	5.83519954617064	8.27641211223826	5.98449811502303
Ga	13.46892013181801	13.68843649456914	6.03441919991914
H	12.70392626423895	8.66726177434287	5.87242509173132
H	1.92580486959095	13.03905168793932	2.77042470227652
H	9.62902514210786	18.48719936962444	2.80454881817771
H	9.62902506201349	13.04046304005587	2.76833076858912
H	9.62902488019899	7.59242100060757	2.73413534147319
H	0.77682482973739	11.44172615164436	3.92960745636118
H	14.62961379713962	11.44172611318524	3.92960795243078
Ga	7.70318642252298	16.32698987457123	3.88384401915447
Ga	7.70324587252328	10.85448502603103	3.90766722179626
Ga	7.70297930057370	5.42486640537787	3.84725149330780
Ga	7.70320294507230	22.06481331639581	3.58570511056465
Ga	3.80658042423567	16.34106808000618	3.87489280669515
Ga	3.82109437967683	10.88362310509712	3.85491885771463
H	4.62962024127525	5.99564051977949	3.89357735179999
Ga	11.59981648630584	16.34106739830900	3.87496920508826
Ga	11.58545974021146	10.88355891498829	3.85494806860531
H	10.77682053319840	5.99563919315589	3.89357711498538
Ga	1.93777368972204	13.68877393314658	6.03444720378515
H	2.70251341859411	8.66726132865075	5.87242543978329
H	8.84784098281057	3.22350892003083	5.83627572908351
Ga	9.65767411062484	19.06781368208297	5.91346587888716
Ga	9.62251737613303	13.62953950467351	5.94287704179949
Ga	9.57104556099839	8.27632519384385	5.98451860403687

H	0.74840065691447	11.67346249059091	7.64098895550732
H	14.65803976851663	11.67346261158736	7.64098959831196
Ga	7.70318706698889	16.67518536173699	7.50848583183731
Ga	7.70290702033899	10.31829137999404	8.68668431544318
Ga	7.70307308976022	5.78012725414260	7.57010939621969
Ga	7.70324775475873	22.23427638765218	7.46312213340231
Ga	3.89784801050662	16.73844065300541	7.47889819034825
Ga	3.66083577187972	11.20450318448985	7.55576053849169
H	4.60139090138104	6.22734726357780	7.60533348121443
Ga	11.50884557160250	16.73815087656638	7.47864414078726
Ga	11.74532656293253	11.20447860333521	7.55560061288614
H	10.80504969425944	6.22734634405519	7.60533302697177
P	5.78226846341140	17.68820050628307	3.97753471069781
P	5.76864373408451	12.27159318813019	3.96512008619396
P	5.76719046763271	6.85826487202245	3.96216684730178
H	6.38704565173519	22.71684348225099	4.00420325773135
H	12.85194069118234	17.25642361455393	3.96807756460949
P	13.48596471911481	12.29280405246072	3.98892368397021
P	5.81902222924972	17.89831802425028	8.08310527876765
P	5.78431369362891	12.15768980670514	7.84746541448852
P	5.72675573732658	7.01083449572291	8.00678044467555
H	6.39778602416292	22.90385776008191	7.89512874956660
H	12.85064284612142	17.45114195178271	7.85597208581115
P	13.59123551741055	12.47900016621592	8.11259302650657
H	7.70321977560076	4.53002835960378	2.61196076086100
H	7.70321997315921	20.84237162156107	2.68056181578856
H	7.70322003272666	15.40326639313142	2.65531099983950
H	7.70321992585601	9.95986313273881	2.62421712201760
H	3.85161008495934	15.39798393967427	2.64793619352444
H	3.85160995754089	9.96381134771977	2.62972784446498
H	11.55483001683044	15.39798434626515	2.64793740535065
H	11.55482989065023	9.96381195356887	2.62972867491072
H	2.55450143760943	17.25642183432721	3.96807763178558
P	1.92047408501955	12.29283671729263	3.98893012092554
P	9.62417053067806	17.68814426600365	3.97746925687920
P	9.63788163321859	12.27155932317825	3.96511520642985
P	9.63913781978537	6.85805365053294	3.96203267022460
H	9.01939442735150	22.71684277236692	4.00420264486526
H	0.63926647604667	14.47657184706328	5.89317725870910
H	14.76717404848361	14.47657317507619	5.89317638140723
P	7.70318687022141	4.06937213736724	5.86912293522510
P	7.70316821447506	20.36657193821263	6.04127587318394
P	7.70321216180313	14.99152656087395	5.90126543050168
P	7.70316104538754	9.70762806886489	5.98820000513111
H	4.48384876127513	19.92840938556246	5.92900078500303
P	3.88721268080746	15.01279073751534	5.90466221204552
P	3.80842355866450	9.55086436287341	5.87732029483390
H	10.92259281946848	19.92841070330569	5.92900146288388
P	11.51942256196769	15.01256884870371	5.90459177517098

P	11.59790094232867	9.55064986716075	5.87724015041240
H	2.55579684419458	17.45114104225961	7.85597160450269
P	1.81504906955176	12.47920214303348	8.11259997040026
P	9.58750880882786	17.89813952390547	8.08282417945122
P	9.62194669557412	12.15763260244798	7.84738080066200
P	9.67947410915657	7.01061676533726	8.00673343017385
H	9.00865287014752	22.90385823552664	7.89512904586292
H	5.39470283145282	13.11619479432353	8.81709749947380
H	10.01193347819812	13.11620018249204	8.81682929298507

4) Adsorbed H_2^+ *

H	5.77741506522534	18.48719924805338	2.80454896761490
H	5.77741491745663	13.04046331321048	2.76833025992228
H	5.77741486106292	7.59241997060365	2.73413671783297
H	13.48063516000035	13.03905253010322	2.77042349244850
H	6.55859764993924	3.22350858411778	5.83627545150464
Ga	5.80272421869195	19.12576160728170	5.98427214769717
Ga	5.78635133496740	13.63150488826907	6.01622776363905
Ga	5.77827490065174	8.25277069870296	5.96979153696967
Ga	13.46360026128720	13.69272487852874	6.02593582491909
H	12.70392627225688	8.66726178857584	5.87242509936988
H	1.92580492239422	13.03905172411688	2.77042470031318
H	9.62902523471192	18.48719937109050	2.80454882867393
H	9.62902505330170	13.04046300345780	2.76833078505241
H	9.62902482659151	7.59242104143665	2.73413532816083
H	0.77682480107534	11.44172611751295	3.92960748030775
H	14.62961381859655	11.44172610278300	3.92960796075506
Ga	7.69518404760356	16.35629943394692	3.87188370686744
Ga	7.68076075435529	10.91166557042502	3.85496864135356
Ga	7.70281398479898	5.41708245344395	3.85078101802427
Ga	7.70320938061170	21.84567839116242	3.88458810165718
Ga	3.82590371270188	16.35363572665010	3.87565111965322
Ga	3.82733337576859	10.88471888376110	3.86077338303684
H	4.62962030586126	5.99564059858528	3.89357731544229
Ga	11.57697100560686	16.36360286654866	3.86795750163960
Ga	11.58324954591743	10.89218411545321	3.84671166065365
H	10.77682058058994	5.99563914019547	3.89357712418921
Ga	1.94603961471315	13.69442531500259	6.03741459823368
H	2.70251338973995	8.66726129103778	5.87242541066085
H	8.84784109830293	3.22350887468461	5.83627572084217
Ga	9.60086256342531	19.12896848200658	5.98140335939806
Ga	9.61512994998923	13.69390447418985	5.90943883840296
Ga	9.60349654694742	8.25115108608138	5.98499945594101
H	0.74840072342168	11.67346251167858	7.64098897841702
H	14.65803979817190	11.67346259930183	7.64098959853229
Ga	7.69845780313869	16.67791612962859	7.53527375562434
Ga	7.50056522033058	10.78313373335484	8.03610197540272
Ga	7.69947769996148	5.78258408682001	7.56963452573626
Ga	7.70324797938070	22.19288837068215	7.44579637450772

Ga	3.90822935670717	16.72744694408760	7.48842150342302
Ga	3.74155720299109	11.25014793905089	7.59881006681035
H	4.60139082729093	6.22734723121805	7.60533347010012
Ga	11.49166506087596	16.74349635814933	7.49583152404047
Ga	11.76007554373979	11.18048534421831	7.57268019251513
H	10.80504970649867	6.22734634342860	7.60533302259556
P	5.78055469014719	17.72242742348039	4.00494732752560
P	5.75593685143837	12.29827369160679	3.98413871748234
P	5.76834294464335	6.85145038340176	3.95636709453056
H	6.38704560179643	22.71684344140643	4.00420322920576
H	12.85194063107259	17.25642355025771	3.96807747251219
P	13.48663067421232	12.29322936096169	3.98810799928713
P	5.80834682650887	17.88373213794722	8.10470603794093
P	5.71636096626311	12.40617264369482	8.06780457077728
P	5.72532490544203	7.01587002189717	8.00370254324060
H	6.39778605522883	22.90385779911781	7.89512871849444
H	12.85064295387106	17.45114198450514	7.85597212307908
P	13.58964733315879	12.48387768986194	8.11155069088171
H	7.70321982271281	4.53002838042390	2.61196076991095
H	7.70322003178869	20.84237179428868	2.68056197102218
H	7.70322003184816	15.40326639608399	2.65531093801233
H	7.70321999773000	9.95986312646933	2.62421694870900
H	3.85161010161624	15.39798397399591	2.64793626513905
H	3.85160996121045	9.96381137681294	2.62972787444867
H	11.55483003924240	15.39798444734707	2.64793751385782
H	11.55482987154927	9.96381196166443	2.62972869373670
H	2.55450143826114	17.25642183177332	3.96807759230483
P	1.92108768527414	12.29330900416018	3.99010648459552
P	9.61771483569932	17.72043490849925	4.00491564293385
P	9.63794336837605	12.28006458952538	3.96672027798612
P	9.63801292921806	6.85353844003633	3.95849644517959
H	9.01939438757532	22.71684269325570	4.00420259487898
H	0.63926639088586	14.47657189464604	5.89317720215736
H	14.76717406090011	14.47657319125503	5.89317637732221
P	7.70312948745495	4.06860647653117	5.87172287543443
P	7.70160589080726	20.48181976155921	5.90317779036742
P	7.69004635824419	15.01574901310345	5.89410357545347
P	7.69423820435288	9.63055514720204	5.86732340961876
H	4.48384900012508	19.92840926546644	5.92900073337003
P	3.88699669792883	15.01790574187441	5.89468907858619
P	3.79993575088825	9.57048969373084	5.89762245055988
H	10.92259265868248	19.92841063083014	5.92900141626377
P	11.53045757852440	15.02682530623757	5.90261233243914
P	11.60099081332631	9.55443729530166	5.87159191239954
H	2.55579670405496	17.45114109247066	7.85597165441593
P	1.82565834867556	12.47216034352135	8.10485780485476
P	9.58904763329692	17.88613757071423	8.10913174176760
P	9.61491532148055	12.14880959259605	7.78200103474781
P	9.67950895433142	7.01026421385588	8.01075848890921

H	9.00865284875719	22.90385821076032	7.89512902999720
H	9.79998709753335	13.04001390621270	8.85966440165888

5) Bare cluster + 1H₂O-OH*

Energy=-8418.443830039158

H	5.77741507815028	18.48719918849855	2.80454893179712
H	5.77741486075981	13.04046332162871	2.76833024402791
H	5.77741491943842	7.59242006589461	2.73413664933337
H	13.48063524342842	13.03905248816196	2.77042348991341
H	6.55859720189289	3.22350857096591	5.83627545234088
Ga	5.80185507515387	19.11784727301812	5.98037683444357
Ga	5.75839973487640	13.69812180380503	5.94374299528404
Ga	5.75861700475588	8.21694228428827	6.00493325850540
Ga	13.45706688459531	13.68882637632837	6.03714982392586
H	12.70392628208568	8.66726178748618	5.87242508403179
H	1.92580485824628	13.03905173626501	2.77042461726167
H	9.62902517110152	18.48719932092787	2.80454883658176
H	9.62902508143375	13.04046303147222	2.76833079000901
H	9.62902479323619	7.59242104940221	2.73413537038509
H	0.77682480800672	11.44172610667687	3.92960747318531
H	14.62961374814162	11.44172615992640	3.92960794474766
Ga	7.71460494915394	16.35413232461193	3.87373928015805
Ga	7.69175141993923	10.91118270408183	3.86026298230540
Ga	7.69507208868367	5.38433486290290	3.88871065457851
Ga	7.70327350157854	21.84177267119422	3.88922700613727
Ga	3.82422178745112	16.35916817753120	3.87113468618367
Ga	3.83129829048811	10.86165103085553	3.88970446377605
H	4.62962023860549	5.99564053737817	3.89357729567140
Ga	11.57697599483240	16.34761162537734	3.88467135518582
Ga	11.56039824243092	10.88271015914832	3.86464026956892
H	10.77682058908291	5.99563916559455	3.89357706229674
Ga	1.94509150772199	13.65959841432701	6.06990771166118
H	2.70251359219967	8.66726148138444	5.87242542671849
H	8.84784153425318	3.22350883057768	5.83627572884658
Ga	9.60361315023792	19.12035688164339	5.98617445651372
Ga	9.59725032586372	13.63594832795275	6.03011894184367
Ga	9.58619829800758	8.20150872502930	6.01214606532072
H	0.74840063632520	11.67346247355550	7.64098896690841
H	14.65803976098142	11.67346263242917	7.64098960179976
Ga	7.69791190018149	16.66122942801167	7.51661879784627
Ga	7.56993689639062	11.12332803017896	7.67341708680656
Ga	7.70758099999722	5.45195308322498	8.01286546705133
Ga	7.70312586819271	22.18932442602905	7.44419838878152
Ga	3.90731493725868	16.72554231155088	7.47356709326648
Ga	3.84395969758990	11.07908826873404	7.81740710438102
H	4.60139069218135	6.22734716467843	7.60533346157588
Ga	11.49467648472185	16.72500912930238	7.48994974312094
Ga	11.61982070057466	11.20438168636752	7.55954397697280
H	10.80504980093363	6.22734635114113	7.60533299568923

P	5.78742507316875	17.71707160875052	4.00057704789941
P	5.75364791800733	12.29542523694627	3.97598786262320
P	5.77488249731409	6.84712986408601	3.95813979258285
H	6.38704561675872	22.71684346176369	4.00420321444869
H	12.85194066178281	17.25642361857373	3.96807757242799
P	13.47897572612327	12.28795355759937	3.98812093621201
P	5.81011179528867	17.87694277334890	8.10111313823999
P	5.72179545230160	12.53711449792099	7.94623616187661
P	5.77342229799265	6.94965044117185	7.97446843326035
H	6.39778613061382	22.90385780945216	7.89512871842360
H	12.85064296577699	17.45114199240526	7.85597213988572
P	13.54370762619146	12.44297276841671	8.08670767812493
H	7.70321984127821	4.53002837662587	2.61196088294303
H	7.70322003739467	20.84237178259288	2.68056193939187
H	7.70322006387736	15.40326650917973	2.65531100508563
H	7.70321995279782	9.95986304126144	2.62421695462267
H	3.85161005553340	15.39798402942547	2.64793624325661
H	3.85160999696117	9.96381137698845	2.62972790718486
H	11.55483003482335	15.39798434680170	2.64793739152451
H	11.55482987073710	9.96381200599755	2.62972873751604
H	2.55450150876887	17.25642177166729	3.96807760935422
P	1.92690774705855	12.28946706579207	3.99086535981669
P	9.62601510096433	17.72307309974577	4.00300447148059
P	9.63629997580361	12.29639905342809	3.98688035461622
P	9.62503915057654	6.84165075546927	3.95522656579860
H	9.01939435214482	22.71684268908516	4.00420261119327
H	0.63926654878517	14.47657186278149	5.89317727100192
H	14.76717397660907	14.47657311708371	5.89317634960325
P	7.70513558724534	4.08504202703516	5.91568861593596
P	7.70245687257527	20.47767891264265	5.90369697665058
P	7.70274147391370	15.02405729474155	5.86506812828443
P	7.67960672276469	9.59812241281252	5.84075154037072
H	4.48384900762451	19.92840927263673	5.92900073131363
P	3.85098770420251	15.04226648426175	5.86719482232078
P	3.80323045754803	9.57930571334562	5.90870708854628
H	10.92259262800162	19.92841059533235	5.92900143517419
P	11.51193217158165	15.00727951528201	5.90420934499718
P	11.57848855351843	9.53657263804549	5.87289342988217
H	2.55579671242863	17.45114108221470	7.85597164755888
P	1.87910286027912	12.42147342318614	8.08676584178098
P	9.58916519021166	17.87545360209619	8.10370586719722
P	9.61541440938633	12.31998995194443	8.05406723887986
P	9.65344788257038	6.98146166962698	8.00472785150293
H	9.00865278525881	22.90385820623306	7.89512904125052
O	4.34892953145035	9.84620465112665	9.24770403987489
O	6.92118706506305	9.83621993911268	9.20489389095375
H	4.13095162168674	10.25946206906731	10.09890457018731
H	5.87326392925379	9.80080525658279	9.22831090194377
H	7.21461721393354	8.91038971872002	9.18053742783731

6) Adsorbed $H_1^+ + 1H_2O-OH^*$

Energy=-8418.913770660403

H	5.77741509913087	18.48719917748738	2.80454893686859
H	5.77741492950711	13.04046336922068	2.76833019098885
H	5.77741490751392	7.59242005698622	2.73413665467940
H	13.48063516317962	13.03905253844266	2.77042347575173
H	6.55859712803095	3.22350852338685	5.83627545648531
Ga	5.80514587995215	19.12724917525336	5.97772512410046
Ga	5.77356335124372	13.78184250218587	5.81312078541031
Ga	5.76272523670716	8.19253560307472	6.00989796633963
Ga	13.46054619800066	13.68754655876348	6.03920928719084
H	12.70392630315899	8.66726176879075	5.87242507913674
H	1.92580495469126	13.03905181012124	2.77042458997205
H	9.62902518705739	18.48719930491313	2.80454881018787
H	9.62902506611870	13.04046304084476	2.76833078618846
H	9.62902485077822	7.59242099840991	2.73413539621854
H	0.77682474586490	11.44172603638290	3.92960751793003
H	14.62961382741616	11.44172609090799	3.92960796366786
Ga	7.72437198551083	16.37031703321202	3.86008986347942
Ga	7.71533885964449	10.91196784355485	3.85556321264297
Ga	7.69550413735481	5.37454060430249	3.89296570203128
Ga	7.70333081410420	21.84535245463261	3.88490547206829
Ga	3.82399043176765	16.36984733443894	3.86052883696363
Ga	3.81385625837876	10.86100994893109	3.88597107644971
H	4.62962025814352	5.99564055777921	3.89357730533381
Ga	11.58022356349715	16.34814581699062	3.88139536899883
Ga	11.57472838753606	10.87995712932546	3.86389799230645
H	10.77682052568896	5.99563921191884	3.89357705228523
Ga	1.93935175357762	13.65421624541730	6.05769842568446
H	2.70251347372136	8.66726134332212	5.87242541951796
H	8.84784158506249	3.22350885203511	5.83627574388545
Ga	9.60352736618638	19.12712754080889	5.98717130223800
Ga	9.61058749742110	13.63113692035404	6.02786980333168
Ga	9.60540517811308	8.17790472408698	6.00043364643162
H	0.74840064298942	11.67346249747867	7.64098896265552
H	14.65803975896148	11.67346262765992	7.64098960771897
Ga	7.70536002726580	16.68396371482526	7.52910098620900
Ga	7.72375376570066	11.01695859444106	7.70301164914029
Ga	7.70562594699891	5.46139897296364	8.02409313838256
Ga	7.70310735793347	22.19243698310643	7.44548269933791
Ga	3.91205415384517	16.74605928992044	7.48165613708125
Ga	3.69962825511646	10.98104610264420	7.85413922522058
H	4.60139084612667	6.22734724193346	7.60533347370207
Ga	11.49594681773154	16.72754477311056	7.49394613087528
Ga	11.64420388959470	11.19448534196077	7.57190489982912
H	10.80504971243275	6.22734637259116	7.60533300959980
P	5.78999266811151	17.71899631648111	4.00192966589471
P	5.75799018988947	12.28005537028919	3.95851799906523

P	5.77637776902557	6.84369356812524	3.95612061102950
H	6.38704575971139	22.71684342469182	4.00420318807190
H	12.85194060347766	17.25642354458251	3.96807753513237
P	13.48261424737648	12.29080867817169	3.98918354212971
P	5.81390036032435	17.88697766300327	8.10774303895938
P	5.72629461825365	12.31127529461535	7.64415270863430
P	5.76199978724671	6.96337720355888	7.99432987586852
H	6.39778587666422	22.90385778829270	7.89512876607985
H	12.85064300280327	17.45114200259853	7.85597216103840
P	13.55160042848639	12.44753948658616	8.09304015907409
H	7.70321984173353	4.53002833743051	2.61196078177724
H	7.70321995796804	20.84237179832358	2.68056192880053
H	7.70322005874113	15.40326650978675	2.65531097287224
H	7.70321993895509	9.95986307238517	2.62421704198837
H	3.85161006558748	15.39798400325514	2.64793621591877
H	3.85160996812877	9.96381138820463	2.62972794496736
H	11.55483006704940	15.39798442053912	2.64793743842434
H	11.55482987967853	9.96381198946691	2.62972871685460
H	2.55450148782412	17.25642179275940	3.96807763015319
P	1.92320476146680	12.29080136753439	3.98932553174452
P	9.63281323566346	17.72816205948243	4.00473057791135
P	9.64691853291785	12.29697534858748	3.98739351287845
P	9.62351452038538	6.83537518464259	3.95012172027866
H	9.01939431518850	22.71684267331936	4.00420261127194
H	0.63926645507669	14.47657185545849	5.89317726106024
H	14.76717403354583	14.47657315499712	5.89317634375210
P	7.70449529344412	4.08609855834722	5.92284757217505
P	7.70407758725813	20.48197882236442	5.90268334418261
P	7.72914373584872	15.04266461301942	5.87221115834535
P	7.69118520803250	9.57392771265536	5.83053736808666
H	4.48384895450327	19.92840930993761	5.92900072070645
P	3.84053243878469	15.05350649055487	5.87646137129495
P	3.80377340229453	9.56821697620992	5.91130931890098
H	10.92259260121337	19.92841057898040	5.92900143013604
P	11.51501458876987	15.00851383272058	5.90744130197814
P	11.58038692494785	9.53811546801184	5.87531142416927
H	2.55579677635713	17.45114106089299	7.85597163148019
P	1.85821750985342	12.44178532503135	8.09724949374346
P	9.59652581949309	17.88624403866735	8.10810413064853
P	9.64565515179205	12.33726735241521	8.07616523236563
P	9.65734525685128	6.98757613738910	8.00612470573929
H	9.00865301807565	22.90385828034052	7.89512907302219
O	4.36605661421273	9.93565995291762	9.33415222596640
O	6.94192089564111	9.88303740604061	9.26481235481078
H	5.76441638700469	13.14725875475610	8.77788976107855
H	4.13603246297109	10.37476696823763	10.16824678196710
H	5.89564237222529	9.86933396327710	9.29324450341972
H	7.23228941736888	8.95828386383793	9.33555996081063

7) Bare cluster + 2H₂O-OH*

Energy=-8570.822481123916

H	5.77741509355736	18.48719917234178	2.80454892070445
H	5.77741495341246	13.04046342364422	2.76833018261746
H	5.77741496560003	7.59242010056595	2.73413664818872
H	13.48063510309013	13.03905259615285	2.77042343901295
H	6.55859739972383	3.22350855946816	5.83627543915562
Ga	5.79873237504365	19.10806486440624	5.97365911248960
Ga	5.74328627853658	13.73731254135377	5.94220093714020
Ga	5.75276177051156	8.22100731317197	6.00463358149615
Ga	13.44935061980973	13.69544528188669	6.03304328106067
H	12.70392628963688	8.66726178246693	5.87242503813402
H	1.92580497588752	13.03905184358306	2.77042456737557
H	9.62902511305711	18.48719933130717	2.80454885729843
H	9.62902508490099	13.04046307173932	2.76833079286611
H	9.62902481490198	7.59242104255610	2.73413538118496
H	0.77682473162673	11.44172600876707	3.92960753756215
H	14.62961387203645	11.44172602071024	3.92960799215525
Ga	7.70490309110247	16.34749693188591	3.89403769647074
Ga	7.68371218207167	10.92224707328669	3.85452332547524
Ga	7.69271822463399	5.38589699187128	3.88838740276465
Ga	7.70866414731701	21.83603424459669	3.89676917378347
Ga	3.82641118540745	16.33881789490922	3.91201803474981
Ga	3.82887107018472	10.87631034351273	3.88585591868095
H	4.62962019324770	5.99564051233251	3.89357729556080
Ga	11.56494285474959	16.35183723367068	3.89073640652276
Ga	11.54760143400664	10.88911850516081	3.86407476887451
H	10.77682057714290	5.99563917012563	3.89357706289134
Ga	1.98782734949202	13.71400514286439	6.09470494630440
H	2.70251344868805	8.66726131350122	5.87242540944987
H	8.84784133605768	3.22350890403870	5.83627572326606
Ga	9.59553788202269	19.09364877927999	6.03651260503589
Ga	9.55727455944740	13.67390157003372	6.03799740966028
Ga	9.59249794193348	8.19518872834733	6.00481984476229
H	0.74840064549808	11.67346250188945	7.64098897829443
H	14.65803972059015	11.67346262669673	7.64098961730595
Ga	7.57580701870137	16.57348721078034	7.73604327000109
Ga	7.57769604745245	11.09385437077225	7.63062853513654
Ga	7.70709093177256	5.45438449590314	8.01165249933743
Ga	7.70272544997155	22.18006596664805	7.42905836491138
Ga	3.95435077933603	16.61695991513827	7.79771305587099
Ga	3.83004271900359	11.07576257378551	7.82045370918896
H	4.60139083183060	6.22734723837101	7.60533346976264
Ga	11.48265125667034	16.71689875227769	7.51330281030355
Ga	11.60805269986889	11.21676296691221	7.55025840421669
H	10.80504974177710	6.22734634321277	7.60533301471810
P	5.78230200857052	17.71732563972302	3.99755781309961
P	5.74980287328696	12.30744396422693	3.98267190167186
P	5.77313681253814	6.84796425825216	3.95878424353367

H	6.38704549526915	22.71684348301449	4.00420321449492
H	12.85194062084812	17.25642354509915	3.96807752509596
P	13.47674298639673	12.28666615944785	3.98771586914992
P	5.80801334530037	18.04645763566228	8.04796896967224
P	5.73676657997019	12.47878151936540	7.89548315888495
P	5.77266570626160	6.95025943270818	7.97325614052051
H	6.39778612560640	22.90385789948188	7.89512875009000
H	12.85064293923768	17.45114205518011	7.85597217074739
P	13.54093135105860	12.44335483897442	8.08168125962835
H	7.70321980222656	4.53002830179640	2.61196084403717
H	7.70322008490850	20.84237175094677	2.68056191846593
H	7.70322006957910	15.40326649416836	2.65531099380559
H	7.70321992421487	9.95986300838080	2.62421701941996
H	3.85161004987506	15.39798400334242	2.64793619491241
H	3.85160995936706	9.96381135870993	2.62972794373727
H	11.55483007649689	15.39798445202585	2.64793745884321
H	11.55482988802435	9.96381195974742	2.62972875128720
H	2.55450151996561	17.25642177093572	3.96807765659125
P	1.92240186797934	12.30278842902071	4.00166902083795
P	9.61867630836164	17.72633383240403	4.01006901865351
P	9.62852671213271	12.30842419417794	3.99483352291566
P	9.62542261031008	6.83877862842056	3.95312695541834
H	9.01939440497033	22.71684273146824	4.00420262714482
H	0.63926645188506	14.47657186048509	5.89317725516510
H	14.76717412048496	14.47657320997582	5.89317632727106
P	7.70507246911081	4.08498038234799	5.91507918348752
P	7.70853259164856	20.47926833420441	5.88424401823355
P	7.68002878489768	15.07731314961630	5.89998962135819
P	7.68685554270541	9.57391346106014	5.81450247993185
H	4.48384901973952	19.92840927164825	5.92900072606642
P	3.86847963125473	15.11387314390613	5.93065143571267
P	3.79861340164851	9.58360594130733	5.90526461892252
H	10.92259274906985	19.92841041507164	5.92900134529178
P	11.50519903310911	15.00707516172904	5.90994176698802
P	11.57833093501417	9.53767342685468	5.87067626980714
H	2.55579664360046	17.45114110279840	7.85597167391815
P	1.87409094528870	12.42804069510785	8.09351337453248
P	9.56214423044313	17.82120764315924	8.13666727664002
P	9.59875869564787	12.31570137592435	8.04595646271445
P	9.65362573018539	6.98196078177678	8.00230977361053
H	9.00865277964099	22.90385816910861	7.89512905710035
O	4.33471676906104	9.84006481232324	9.24865992226555
O	6.92528647760370	9.82129316066895	9.19531200627104
H	4.14156696358583	10.26804576116116	10.09846800793065
H	5.88291854957698	9.79224656803844	9.21773502115736
H	7.21126073714641	8.89302705684598	9.18069521423463
O	4.32670613444947	15.42648202237796	9.31921561660394
O	6.91022902219645	15.21130050639900	9.24360314042030
H	4.18258310624636	15.95478455818629	10.12114061607197

H	5.87169387836117	15.30939863567152	9.29503047777271
H	6.99612037803882	14.26946306670258	8.98482491986211

8) Adsorbed $H_1^+ + 2H_2O - OH^-$

Energy=-8571.298061233267

H	5.77741508299260	18.48719915140247	2.80454893158808
H	5.77741496347862	13.04046340365072	2.76833020474871
H	5.77741492689120	7.59242007567928	2.73413664262680
H	13.48063509362222	13.03905260502205	2.77042344117582
H	6.55859731482578	3.22350850553678	5.83627544516405
Ga	5.79529762137517	19.11010000504145	5.97511869854686
Ga	5.74990757852824	13.83429459449543	5.81292514912658
Ga	5.75886889091543	8.19823721367943	6.00829536338110
Ga	13.45205728855176	13.69516828676419	6.03416348594818
H	12.70392630480634	8.66726172196749	5.87242508662737
H	1.92580498560499	13.03905185778592	2.77042456116596
H	9.62902511260973	18.48719932105428	2.80454884196027
H	9.62902505616058	13.04046309008890	2.76833077551820
H	9.62902483732221	7.59242102040522	2.73413538424567
H	0.77682471036078	11.44172599787854	3.92960755604163
H	14.62961387543591	11.44172602068947	3.92960799499037
Ga	7.71627464415758	16.36520659146390	3.87730250657683
Ga	7.70333976104742	10.92404530320783	3.85091851142549
Ga	7.69503382353381	5.37513858724512	3.89288574596431
Ga	7.70809207619856	21.83763426733855	3.89492829341892
Ga	3.82547920066361	16.35506668908992	3.89240909848411
Ga	3.81344173459798	10.87781402810408	3.87990382054240
H	4.62962027294884	5.99564056743243	3.89357732031946
Ga	11.56792406504670	16.35303926651278	3.88684651559569
Ga	11.56263897124792	10.88639022333149	3.86339704899369
H	10.77682053979219	5.99563919707188	3.89357707236300
Ga	1.98285623608581	13.70911551144513	6.07760886055482
H	2.70251345196671	8.66726134229977	5.87242543470034
H	8.84784140467818	3.22350892095425	5.83627574083339
Ga	9.59514324681076	19.10341630122364	6.03497842341464
Ga	9.56441795631398	13.67426784876268	6.02609873314792
Ga	9.60414321545394	8.18110885892049	5.99886610831766
H	0.74840065417790	11.67346250073770	7.64098897355267
H	14.65803972448163	11.67346262343061	7.64098961408838
Ga	7.59008510738120	16.60360301342980	7.74281305993453
Ga	7.70175533585764	11.02313446388231	7.68747132416304
Ga	7.70459460186785	5.46499926280682	8.02360161941001
Ga	7.70265553510460	22.18193043209784	7.43107583771775
Ga	3.96342703849068	16.61140605373777	7.81484917503976
Ga	3.69090921429157	10.98861809641300	7.83189906039893
H	4.60139086318556	6.22734723797047	7.60533348498604
Ga	11.48300766081317	16.72246236090163	7.51543194604370
Ga	11.62781843031554	11.21258685182030	7.56788923196139
H	10.80504967966120	6.22734637210876	7.60533300879890

P	5.78524232820142	17.71895023583593	3.99745214564980
P	5.75379363790550	12.29672451142228	3.96810695440808
P	5.77583972899374	6.84440696368857	3.95604462007964
H	6.38704550015065	22.71684347768423	4.00420321449394
H	12.85194062446711	17.25642353369197	3.96807752461179
P	13.48052763032955	12.28960854454329	3.98860336505630
P	5.80303194054745	18.04857726693664	8.05461217581334
P	5.70665503022848	12.30315740078719	7.60571019047098
P	5.76027476495947	6.96594116201741	7.99258128354652
H	6.39778613551207	22.90385788869351	7.89512873974851
H	12.85064294488110	17.45114201941816	7.85597212980459
P	13.54886389094993	12.45042660961900	8.08802405010012
H	7.70321980744420	4.53002829095422	2.61196075817770
H	7.70322007967950	20.84237174528706	2.68056190735117
H	7.70322007976197	15.40326648845981	2.65531097943193
H	7.70321992632911	9.95986303690232	2.62421706155791
H	3.85161004461951	15.39798401374437	2.64793619038487
H	3.85160996931444	9.96381131603241	2.62972787357731
H	11.55483007217689	15.39798444723827	2.64793745505928
H	11.55482989901420	9.96381194321662	2.62972869539882
H	2.55450153003881	17.25642176616782	3.96807766207777
P	1.91850218066901	12.30369483096902	3.99965868436233
P	9.62588845643475	17.73246547409808	4.01118964889424
P	9.63834078649142	12.30700849193403	3.99379437025103
P	9.62359784258532	6.83567905430931	3.94979802156237
H	9.01939439476193	22.71684271561688	4.00420262713914
H	0.63926644389551	14.47657187531876	5.89317726588256
H	14.76717413568882	14.47657323210427	5.89317634987547
P	7.70428188100362	4.08542676704863	5.92204524551817
P	7.70504809914567	20.47975180721027	5.88612924790804
P	7.70338292635577	15.10180528360955	5.89964358068137
P	7.68995127195291	9.57270346012399	5.82424970145943
H	4.48384901807683	19.92840928878321	5.92900072040958
P	3.84845407428485	15.13288236042055	5.91881882141128
P	3.79951637202513	9.56929470505730	5.90231087673309
H	10.92259274987734	19.92841052144624	5.92900142968382
P	11.50664351728343	15.00845885860242	5.91317326267038
P	11.57940005674858	9.54157149798482	5.87623626992833
H	2.55579663156839	17.45114110372788	7.85597167958272
P	1.85418607113619	12.44896141299547	8.10101527921349
P	9.57068779650248	17.83933404360944	8.13600558412781
P	9.61926797273605	12.34866942376559	8.07268804988379
P	9.65800559067266	6.98903881872789	8.00418878204545
H	9.00865277501269	22.90385815861769	7.89512905712212
O	4.36355466445008	9.96120825212166	9.33250970690589
O	6.92820130706779	9.89843034458021	9.26496416196808
H	5.66198331513149	13.10387187069637	8.76118960430465
H	4.12064995249024	10.39635087719634	10.16541730374042
H	5.87674859452032	9.89736129301954	9.29641579084986

H	7.19995048171244	8.96720228056843	9.32832389431378
O	4.45209444588944	15.25684713959437	9.20157536676522
O	6.95943371960613	15.27367467459998	9.23641652391987
H	4.14254433536011	15.52219123963359	10.08139049084156
H	5.87793897138520	15.23271598331302	9.24581453250286
H	7.32190625395293	14.37470587545473	9.21306829232885

9) Bare cluster + 2H₂O-OH* +3H₂O*

Energy=-8800.11157694901

H	5.77741513544342	18.48719921060083	2.80454892603818
H	5.77741492277272	13.04046343909728	2.76833020759051
H	5.77741493154728	7.59242006774570	2.73413668859398
H	13.48063508740405	13.03905260404806	2.77042343527838
H	6.55859741413964	3.22350845992184	5.83627544802955
Ga	5.82607788699827	19.13793340032174	5.95120427616009
Ga	5.75703827107539	13.75478020090319	5.94207808034306
Ga	5.76406511645504	8.23251901091994	6.00500164718983
Ga	13.43271879874643	13.69088346991519	6.03589246610954
H	12.70392630248320	8.66726174705388	5.87242508198567
H	1.92580493460455	13.03905184673136	2.77042455609303
H	9.62902519727502	18.48719932201211	2.80454879824104
H	9.62902506890594	13.04046309467843	2.76833079254986
H	9.62902484731348	7.59242103853493	2.73413536985664
H	0.77682476634492	11.44172602249944	3.92960755913678
H	14.62961389272279	11.44172601964991	3.92960798755601
Ga	7.71031632621859	16.35030299988346	3.89524752231410
Ga	7.68725013031355	10.92473086395160	3.85721015923066
Ga	7.68974042163612	5.38215720122793	3.89090015904830
Ga	7.70994421138000	21.82313990011731	3.91728319267691
Ga	3.83046900574410	16.34374022819852	3.91058248369403
Ga	3.83247445096146	10.87892540118046	3.88640740093911
H	4.62962028141631	5.99564056940613	3.89357731408378
Ga	11.56656228713797	16.34830408443424	3.89576078078879
Ga	11.55359484518317	10.89439832018401	3.86225499374611
H	10.77682055560377	5.99563919088572	3.89357708456600
Ga	1.99213131342264	13.72003761019381	6.09791667423480
H	2.70251343360490	8.66726133272764	5.87242545062781
H	8.84784126454081	3.22350899411772	5.83627574197318
Ga	9.59887262405504	19.07639749665635	6.04126305576448
Ga	9.58639128302536	13.68620909043172	6.02122576571591
Ga	9.61909665827200	8.21949722496486	5.96988392589719
H	0.74840062429590	11.67346247405638	7.64098896779581
H	14.65803973978563	11.67346262312434	7.64098961198360
Ga	7.59350408165209	16.59282015310525	7.74212674588584
Ga	7.58753660506651	11.13771459205690	7.64869875770366
Ga	7.69866175890512	5.47547425753195	8.03154274307804
Ga	7.70455360365843	22.02984593659552	7.63853347698088
Ga	3.95603303409773	16.62850030379398	7.80000250356229
Ga	3.83458436439035	11.08266455980619	7.81721121796515

H	4.60139083560235	6.22734723632195	7.60533344496794
Ga	11.51087008225252	16.59067061567161	7.67734648447297
Ga	11.57133053770355	11.09387267995303	7.69956496968276
H	10.80504975854720	6.22734633979979	7.60533299741340
P	5.78447822806550	17.71847251118509	3.99699967510752
P	5.75232807203996	12.31240805884912	3.98581676100457
P	5.77358115195983	6.85006064377285	3.96042014253851
H	6.38704549435098	22.71684348333738	4.00420322012510
H	12.85194059910528	17.25642353822041	3.96807752766737
P	13.47867531403873	12.28950020742605	3.98767280547782
P	5.81478577576722	18.06225700154007	8.03211282605440
P	5.72935250328898	12.49726309882333	7.89722737941738
P	5.76297247093471	6.96436900365600	7.97904689016911
H	6.39778623615095	22.90385787277301	7.89512873442637
H	12.85064299837611	17.45114200828915	7.85597217195227
P	13.51260225480770	12.41505293508134	8.06111786136808
H	7.70321979225037	4.53002827766150	2.61196078501968
H	7.70322007455133	20.84237174999907	2.68056191757092
H	7.70322004825081	15.40326649278446	2.65531097642080
H	7.70321992806650	9.95986301135288	2.62421705190473
H	3.85161005173797	15.39798401113124	2.64793623205595
H	3.85160999262239	9.96381131362717	2.62972788413578
H	11.55483006133261	15.39798443885598	2.64793745166993
H	11.55482988650281	9.96381196245993	2.62972872709303
H	2.55450148510268	17.25642177894839	3.96807762063578
P	1.92302011094754	12.30373370300013	4.00249558954460
P	9.62498086739371	17.72379339550088	4.00766668970689
P	9.63071231197364	12.30825520119205	3.99255780467266
P	9.62278185455942	6.83576976311093	3.94972469768992
H	9.01939443208291	22.71684272632013	4.00420261679236
H	0.63926641853674	14.47657190791226	5.89317725350069
H	14.76717410150819	14.47657320158795	5.89317635116435
P	7.70599765191370	4.08773419443000	5.92144002145043
P	7.72953651592589	20.49891974678964	5.87883431438025
P	7.69468318645713	15.08899913392012	5.90463103498596
P	7.69953182931274	9.59386424338435	5.83378648031067
H	4.48384901809961	19.92840926136325	5.92900072105193
P	3.87413056685667	15.12331896517877	5.93336141670119
P	3.80024605481179	9.58387143594202	5.90643907587469
H	10.92259257729196	19.92841055946614	5.92900142965635
P	11.51316250142357	15.03621990208612	5.89272350845988
P	11.59321708764237	9.56333388074895	5.85834827446310
H	2.55579676847461	17.45114105088744	7.85597166376083
P	1.87430477589217	12.42817078559817	8.09343838587760
P	9.57841641008774	17.82163670505008	8.13383303601489
P	9.61321551888181	12.36462636743799	8.02883606871091
P	9.67065824572398	7.01090376207689	7.98154736540779
H	9.00865266910908	22.90385814274039	7.89512903060896
O	4.34827296616658	9.85871024026136	9.25460612879295

O	6.93780993162637	9.83807262487107	9.19677351088874
H	4.15078202080680	10.29205549883900	10.10069391140865
H	5.89429697636841	9.81780270311531	9.22328933424049
H	7.20804852333411	8.90594914910901	9.15739457132321
O	4.33873739492493	15.44648210770208	9.32283408646677
O	6.92364207109530	15.22950845119746	9.24665954799925
H	4.20262421802605	15.98077766055154	10.12224830409085
H	5.88552746092975	15.32095680764481	9.29335284867940
H	7.02371029638652	14.28892931149842	8.99192801398211
O	7.71355039366002	20.52423085892830	9.21712395600156
H	8.50365450319107	19.94878396441350	9.10927250730184
H	6.97200894788927	19.89063801707157	9.03248936350537
O	11.61438340850649	15.05326307284178	9.24967951875314
H	10.90404536514071	14.38847893726841	9.11165927314112
H	12.43920072388925	14.52971082056574	9.21026911997607
O	11.31433282865778	9.63841942565756	9.25783218631353
H	10.77916394204150	8.84426901635405	8.99558438893918
H	12.13291020561769	9.29181738796151	9.64931245043211

10) Adsorbed $H_1^+ + 2H_2O-OH^- + 3H_2O^*$

Energy=-8800.58742995038

H	5.77741513100097	18.48719920549302	2.80454892595151
H	5.77741493235867	13.04046343233803	2.76833020457711
H	5.77741493469734	7.59242009976061	2.73413665103165
H	13.48063509839373	13.03905259684413	2.77042343718235
H	6.55859726753770	3.22350850338835	5.83627547587559
Ga	5.82221698839562	19.14219536107078	5.95379695626989
Ga	5.76171354161499	13.85054489636102	5.80955078760845
Ga	5.76847511684387	8.21098993293554	6.00837292006401
Ga	13.43597010558804	13.69067493621072	6.03770318569595
H	12.70392629058096	8.66726175219098	5.87242508848336
H	1.92580495169883	13.03905184104822	2.77042456704006
H	9.62902520251316	18.48719931672231	2.80454880393334
H	9.62902505909728	13.04046308452555	2.76833078554695
H	9.62902483983922	7.59242104066960	2.73413538899284
H	0.77682474722406	11.44172602189930	3.92960755002277
H	14.62961388618330	11.44172602632591	3.92960798746400
Ga	7.72075136620319	16.36942824737013	3.87701875764401
Ga	7.70669783715928	10.92746899340461	3.85235498087071
Ga	7.69229714831280	5.37360715504200	3.89478206145894
Ga	7.70815831788009	21.82362223694199	3.91696875797646
Ga	3.82991907251863	16.36039106382292	3.89083334959851
Ga	3.81576016487105	10.88131162559029	3.87932168632468
H	4.62962025293825	5.99564054451287	3.89357732294901
Ga	11.56965702938383	16.34867206741648	3.89338815960831
Ga	11.56882474277825	10.89131528511761	3.86216134794127
H	10.77682054302327	5.99563919546260	3.89357706984990
Ga	1.98690584956633	13.71536508473098	6.07993462627870
H	2.70251346446549	8.66726135275287	5.87242545351696

H	8.84784141927144	3.22350892951488	5.83627573397002
Ga	9.59878235647977	19.08599990527101	6.04004912548569
Ga	9.59162587794549	13.68740521997102	6.00886840763174
Ga	9.63346140107251	8.20975718663485	5.96698926777021
H	0.74840065012026	11.67346249437295	7.64098896840265
H	14.65803972133073	11.67346263615447	7.64098961172734
Ga	7.60426631679031	16.62220192507829	7.74354248802309
Ga	7.70552400481657	11.06580610207238	7.69855332152146
Ga	7.69570816817660	5.48589925463491	8.04395934158719
Ga	7.70419256222222	22.03274305777463	7.64199431642041
Ga	3.96393176070182	16.62177933729397	7.81755845001377
Ga	3.69289782936644	10.99422939995603	7.83014562701887
H	4.60139074168980	6.22734720660211	7.60533342437500
Ga	11.51232995797795	16.59846528976072	7.68146603338786
Ga	11.59003062756901	11.09356748889829	7.72330813417669
H	10.80504983102238	6.22734632724524	7.60533296785832
P	5.78733112143820	17.72127237998725	3.99751595537410
P	5.75562131967957	12.30114614165460	3.97075647197844
P	5.77583309709490	6.84663824635068	3.95777472903568
H	6.38704549481885	22.71684348295064	4.00420321985811
H	12.85194059493460	17.25642353525517	3.96807752948839
P	13.48247967668145	12.29260769431186	3.98888849932152
P	5.80917875997326	18.06250387690027	8.03928128464151
P	5.69921697603332	12.31834999307986	7.60222423757196
P	5.75075070884560	6.98011979367735	7.99664230048147
H	6.39778624141970	22.90385787280427	7.89512873440432
H	12.85064299820676	17.45114200867328	7.85597217210781
P	13.52097671082243	12.42391565138654	8.06905785827573
H	7.70321982667073	4.53002831672505	2.61196084242787
H	7.70322007446230	20.84237175054924	2.68056191798431
H	7.70322004788886	15.40326649292938	2.65531097221192
H	7.70321992893471	9.95986304111518	2.62421706591458
H	3.85161004002523	15.39798402866677	2.64793623848113
H	3.85160998607385	9.96381131043618	2.62972787495419
H	11.55483006595678	15.39798443615442	2.64793744939083
H	11.55482988853285	9.96381196512703	2.62972870942319
H	2.55450151272252	17.25642176194853	3.96807761998042
P	1.91866314301506	12.30498810665872	4.00064908442196
P	9.63233311284138	17.72987893918062	4.00881940656029
P	9.64102299956714	12.30715981398086	3.99165812926960
P	9.62203357142292	6.83408161887250	3.94763180340063
H	9.01939443177135	22.71684272617221	4.00420261659924
H	0.63926639691854	14.47657189728207	5.89317725999031
H	14.76717409550744	14.47657318933606	5.89317634488054
P	7.70540229618908	4.08789650967855	5.92890575898098
P	7.72663120119593	20.49942984433170	5.88298035275195
P	7.71605024978538	15.11263565635700	5.90080152396409
P	7.70183201160520	9.59139483117628	5.83910511355872
H	4.48384900683929	19.92840927295766	5.92900072065442

P	3.85371707202776	15.14197801964179	5.92117923184621
P	3.79972998858007	9.57090119309935	5.90263828154913
H	10.92259256035344	19.92841054839734	5.92900143497145
P	11.51421082350346	15.03713816531962	5.89935536417073
P	11.59626220809332	9.57009501969277	5.86696295720618
H	2.55579679637489	17.45114103990813	7.85597165844779
P	1.85327550737989	12.45016280217933	8.10139731385206
P	9.58523624099615	17.83637572834426	8.13310536812538
P	9.62605403644181	12.39455361401585	8.05048175333860
P	9.67457608369223	7.01675929261491	7.98391763366035
H	9.00865266387467	22.90385814281069	7.89512903065275
O	4.37844601967230	9.98514422740921	9.34039846864352
O	6.93914559802257	9.91467730849128	9.26629183481536
H	5.64204560791513	13.11669001370917	8.75898782922041
H	4.13070708331515	10.42526958349944	10.16927547502241
H	5.88566898318010	9.92719736096628	9.30391235912073
H	7.18888770440327	8.97591833926362	9.30214714420359
O	4.45326548663981	15.27443669065501	9.20514234222595
O	6.96923899901032	15.27435309448415	9.22780712831335
H	4.16296763130100	15.55878439451311	10.08577105519349
H	5.89348181369227	15.24072736587041	9.23907019318286
H	7.31922815555464	14.37160438129823	9.17256530401478
O	7.71356982805222	20.53514766228461	9.22854427149637
H	8.50092810858089	19.95632367175812	9.12199685919863
H	6.96812422065155	19.90547231005559	9.05510217979108
O	11.64806357825435	15.09812334226724	9.27865062710303
H	10.92828664177070	14.43829995757624	9.20101686020852
H	12.46731088063234	14.56658925904623	9.23552760904557
O	11.28677342178078	9.66337312513504	9.28029973931744
H	10.78515019667680	8.84857214077501	9.01549807892282
H	12.08635661117806	9.35357735054702	9.73693267175839

11) Adsorbed $\text{H}_2^+ + 2\text{H}_2\text{O}-\text{OH}^+ + 3\text{H}_2\text{O}^+$

Energy=-8800.59001328407

H	5.77741509910408	18.48719919365693	2.80454894750932
H	5.77741491426049	13.04046335571103	2.76833025839945
H	5.77741492452668	7.59242008061511	2.73413666312980
H	13.48063510033519	13.03905259734868	2.77042344160748
H	6.55859721472637	3.22350847280842	5.83627542189584
Ga	5.84245672133262	19.20954615384806	5.80840063551862
Ga	5.75825044525081	13.71509708195553	5.93759109115063
Ga	5.76489823603783	8.22804695542110	6.00491992612618
Ga	13.43667508613045	13.68852306448015	6.03948530821723
H	12.70392629387688	8.66726174538346	5.87242506995322
H	1.92580498036414	13.03905186107275	2.77042453539714
H	9.62902517581886	18.48719931570603	2.80454879935235
H	9.62902505342455	13.04046305859593	2.76833079144136
H	9.62902484700870	7.59242105084483	2.73413532956717
H	0.77682470946118	11.44172598338830	3.92960756528832

H	14.62961387965480	11.44172602673028	3.92960798795127
Ga	7.73128565725138	16.34807947889772	3.88917064679944
Ga	7.69210236798346	10.91587039168621	3.85986145040980
Ga	7.69005723668847	5.38035236595081	3.89158389405390
Ga	7.71180809172823	21.83464233942063	3.90563542443605
Ga	3.81469784334365	16.33710334822378	3.90890632415420
Ga	3.83187947489064	10.86768887717004	3.88965254803599
H	4.62962026826504	5.99564055489589	3.89357730948667
Ga	11.57766229737722	16.34198498511220	3.89524619075100
Ga	11.56641612528383	10.88710560989807	3.86303552891443
H	10.77682054008271	5.99563919096666	3.89357709552686
Ga	1.96822567370659	13.68096395695773	6.07693816485191
H	2.70251343805921	8.66726137408670	5.87242543546062
H	8.84784149183524	3.22350890072097	5.83627573772692
Ga	9.60970249922817	19.06245918073156	6.03269149420732
Ga	9.61180030373233	13.64704088674977	6.00388403012909
Ga	9.62053490468432	8.21687540261208	5.97006613069800
H	0.74840069144558	11.67346249655638	7.64098896748959
H	14.65803970721058	11.67346264660314	7.64098961282221
Ga	7.72547172787089	16.45145089270338	7.74592843901767
Ga	7.59244920699326	11.13320999932426	7.65954484642736
Ga	7.69901581046752	5.47481876890522	8.03272417167729
Ga	7.71154575675761	22.05211810570492	7.63975683005737
Ga	3.83592283188790	16.49323284649354	7.81469684123123
Ga	3.83176693216568	11.07932210407322	7.82886147072650
H	4.60139100585241	6.22734729435249	7.60533351448481
Ga	11.52690780282318	16.57626853132811	7.69349615914975
Ga	11.57914971028932	11.08747941075930	7.70727249595572
H	10.80504958224703	6.22734640682290	7.60533305732367
P	5.78752559875612	17.69831019024683	3.97464498088110
P	5.75362366157703	12.29965740284080	3.97779373094134
P	5.77404622508371	6.84932672652671	3.95972060086093
H	6.38704551056477	22.71684347759424	4.00420321461047
H	12.85194059294839	17.25642352826868	3.96807754514475
P	13.48075537698316	12.29121937800206	3.98848578925550
P	5.81691034147373	17.80819349877815	7.70384838189795
P	5.73295386400928	12.49755004384368	7.91020604391182
P	5.76292061500216	6.96434947485710	7.98003386357702
H	6.39778625734874	22.90385785671569	7.89512872369369
H	12.85064302930621	17.45114201401369	7.85597217672976
P	13.51477260022737	12.41549639043378	8.06463227218433
H	7.70321980887823	4.53002826882786	2.61196071306149
H	7.70322007449050	20.84237176643106	2.68056193384328
H	7.70322005327970	15.40326649847506	2.65531099427076
H	7.70321994267353	9.95986303332648	2.62421703279904
H	3.85161007138826	15.39798398186994	2.64793619561679
H	3.85160998365259	9.96381131157751	2.62972784310178
H	11.55483007249277	15.39798442103099	2.64793743333749
H	11.55482989882002	9.96381195800671	2.62972871684223

H	2.55450148234458	17.25642179267936	3.96807764631072
P	1.92533948493233	12.29427877918089	3.99500540767743
P	9.63461139762249	17.72062498046735	4.00489912930916
P	9.63899088014650	12.29266843913758	3.98186545897433
P	9.62256688625954	6.83544908826711	3.94933563608464
H	9.01939441083617	22.71684271044592	4.00420261658899
H	0.63926645381163	14.47657189164385	5.89317727059187
H	14.76717407782745	14.47657317440605	5.89317634073077
P	7.70601384753500	4.08734744972429	5.92250308413543
P	7.75484057664404	20.50860327349512	5.88789352145850
P	7.70910305932054	15.03706128462913	5.87388688104783
P	7.69980764247045	9.59414279254437	5.83944137870163
H	4.48384903327588	19.92840924640860	5.92900073136511
P	3.86189996015407	15.07440640643750	5.91709216013022
P	3.80149803159844	9.58256804136595	5.91207212803531
H	10.92259267035376	19.92841061627070	5.92900142995741
P	11.51227959965614	15.03605905927666	5.89605948055266
P	11.59401901607429	9.56306935913225	5.86117173134684
H	2.55579663786424	17.45114110908658	7.85597167925373
P	1.87347306939757	12.42878040449053	8.09203288914750
P	9.58138967350679	17.81609365915224	8.14819345793851
P	9.62006321824227	12.36342385159941	8.02867027491510
P	9.67129208775814	7.01135266095698	7.98249993698693
H	9.00865265343238	22.90385814291037	7.89512903074307
O	4.35205996511181	9.85887604174488	9.26337587967110
O	6.94031770214812	9.83678954783746	9.20364806838068
H	4.15276239730728	10.28726341799054	10.11156922958033
H	5.89624059340281	9.81636244067098	9.23207605892150
H	7.21229261622158	8.90497117086969	9.16781258763809
H	5.87902517909925	18.64339464626967	8.84029911435310
O	4.34545689638040	15.49949859453758	9.40389774541392
O	6.93386088239717	15.20821603382896	9.26841574940863
H	4.18708844504710	16.07332726851113	10.17070704782884
H	5.90891603270004	15.35847626044841	9.34719970219125
H	6.96171999589849	14.25425672054312	9.03057831054596
O	7.92792504096020	20.64582354984179	9.27634611167017
H	8.49903447951631	19.87703098657660	9.04327774817022
H	7.08763708797451	20.25996814134892	9.57138850109225
O	11.61171473262521	15.04376598267705	9.25156722154309
H	10.91002498635741	14.36968761057376	9.10982731738608
H	12.44289335164646	14.52880256270373	9.23229455436117
O	11.31472355868805	9.63779424286082	9.26309984213321
H	10.78257839164663	8.84137019100785	9.00103659358973
H	12.13010214909038	9.29517651371783	9.66480379248748

12) Co-adsorbed H_1^+* and $H_2^+* + 2H_2O-OH^* + 3H_2O^*$

Energy=-8801.06183262714

H	5.77741508863623	18.48719919998709	2.80454894197467
H	5.77741493226537	13.04046340334953	2.76833019293798

H	5.77741494446867	7.59242009229790	2.73413667068022
H	13.48063509510045	13.03905259991803	2.77042343480267
H	6.55859741680064	3.22350847683974	5.83627545594432
Ga	5.84067171390991	19.21223673607853	5.80971478369739
Ga	5.76065775068486	13.81037304061517	5.80999882119053
Ga	5.76962290971887	8.20586518299467	6.00883205112995
Ga	13.44021288898568	13.68767464842197	6.04115541471217
H	12.70392631209514	8.66726177773166	5.87242508244824
H	1.92580497285808	13.03905185222247	2.77042456159067
H	9.62902518688457	18.48719932704199	2.80454880470927
H	9.62902506425685	13.04046307457450	2.76833078614664
H	9.62902484270103	7.59242104550896	2.73413537933480
H	0.77682472606628	11.44172600041882	3.92960754919005
H	14.62961389105464	11.44172601866957	3.92960798794361
Ga	7.74108183510568	16.36550680998825	3.87289032454345
Ga	7.71132203901984	10.91867125782519	3.85518856443202
Ga	7.69275972853710	5.37183194342828	3.89523706650487
Ga	7.71135557713709	21.83642969680637	3.90374680607026
Ga	3.81470147093970	16.35550864365305	3.88380999097697
Ga	3.81579935579650	10.87011819461442	3.88300403514446
H	4.62962025635010	5.99564054133111	3.89357731974298
Ga	11.58089710111139	16.34213225754004	3.89297529007129
Ga	11.58095063365864	10.88372119603174	3.86321924182907
H	10.77682053939962	5.99563920090357	3.89357707924985
Ga	1.96328477600337	13.67729757243081	6.05897925639668
H	2.70251351773673	8.66726138929664	5.87242542536554
H	8.84784126877210	3.22350901279255	5.83627575816155
Ga	9.60948303453132	19.07194719542854	6.03089949549350
Ga	9.61788118382849	13.64736251619091	5.99593969301031
Ga	9.63577358451500	8.20640407176433	5.96712444189906
H	0.74840065536503	11.67346249362171	7.64098897846538
H	14.65803972519796	11.67346262744998	7.64098961233311
Ga	7.73646255824766	16.47862840774260	7.74901482681453
Ga	7.71247689248024	11.06070161224503	7.70637056964488
Ga	7.69671634337471	5.48441468358750	8.04462145284696
Ga	7.71095761493604	22.05431882752985	7.64418929066799
Ga	3.83819318219808	16.48625868022615	7.81338542773883
Ga	3.69157702829119	10.98771606610600	7.84196789384623
H	4.60139065424221	6.22734714835986	7.60533342286677
Ga	11.52893280232425	16.58358969500724	7.69802483209209
Ga	11.59786097580971	11.08648205456753	7.73125252454391
H	10.80504987697804	6.22734631906592	7.60533296462452
P	5.79056840773845	17.70054124842137	3.97469012879005
P	5.75723399965197	12.28894212438463	3.96315622806471
P	5.77630663058072	6.84588600511717	3.95714083591158
H	6.38704550508740	22.71684348311731	4.00420321451572
H	12.85194059997556	17.25642353408491	3.96807753543864
P	13.48428280804696	12.29403931855727	3.98947363238572
P	5.81032142629068	17.80553353377173	7.71019263491885

P	5.70394322925942	12.31326730915888	7.61956085841239
P	5.75129087008042	6.97880078553897	7.99826065927418
H	6.39778625753913	22.90385786232085	7.89512872384055
H	12.85064303990638	17.45114201249269	7.85597217707508
P	13.52311678339597	12.42398662071931	8.07248330647458
H	7.70321978761527	4.53002827916337	2.61196082510416
H	7.70322007441296	20.84237176102837	2.68056192839596
H	7.70322005305291	15.40326648660383	2.65531097792744
H	7.70321993453964	9.95986302548636	2.62421702173399
H	3.85161006131836	15.39798400242151	2.64793622276334
H	3.85160997652482	9.96381132638642	2.62972790913957
H	11.55483006537368	15.39798442618513	2.64793744521329
H	11.55482988449289	9.96381195509873	2.62972871070216
H	2.55450149751452	17.25642177728547	3.96807763086390
P	1.92112389121505	12.29512813289745	3.99284891976622
P	9.64173716902903	17.72614088685746	4.00616410164895
P	9.64889600002294	12.29236343144392	3.98168065809015
P	9.62196509093667	6.83372859212040	3.94719312233184
H	9.01939441616724	22.71684271577095	4.00420261657231
H	0.63926643548949	14.47657188125613	5.89317725516815
H	14.76717409738298	14.47657319907162	5.89317634682802
P	7.70544243883755	4.08746070222823	5.92903785219763
P	7.75228582942531	20.50980737891937	5.89090040149885
P	7.72935704855447	15.05849276469394	5.87488194969143
P	7.70291244356765	9.59028163282143	5.84371924138340
H	4.48384904979629	19.92840924076883	5.92900073136145
P	3.84085337283910	15.09391539725828	5.89245784184801
P	3.80148013220811	9.56936222737782	5.90843426480379
H	10.92259262335082	19.92841059052193	5.92900142957650
P	11.51331306041673	15.03683068019703	5.90311415029989
P	11.59710984300173	9.56977819815243	5.86991724218048
H	2.55579664810993	17.45114110368472	7.85597167436029
P	1.85409505949257	12.44961348646100	8.09820217680997
P	9.58901482380515	17.83151997341717	8.14813439451175
P	9.63332831770146	12.39288294551046	8.05273129631462
P	9.67496550431633	7.01668403314138	7.98502007686745
H	9.00865265297777	22.90385814272550	7.89512903060566
O	4.38318511902965	9.97976503125211	9.34706265261591
O	6.94559861707953	9.91074880028241	9.27157227391820
H	5.66699671121274	13.14236510179737	8.75513564753227
H	4.13432669673153	10.41391637139183	10.17875699974435
H	5.89250066850180	9.92179316049714	9.31069686410452
H	7.19801774434087	8.97282552764992	9.31155736537159
H	5.86666306748264	18.63998768484363	8.84685069509901
O	4.43793430936268	15.27686793101336	9.22970983727612
O	6.96673309051277	15.30936491252820	9.30342184834231
H	4.06595972233681	15.48781320586742	10.09927250971331
H	5.90056246990431	15.27399833862526	9.30480076432081
H	7.31777440673178	14.41316735228490	9.42342584033376

O	7.92100945682922	20.65363147050291	9.28370431732859
H	8.49346116341261	19.88437123021172	9.05854751030923
H	7.08142487186641	20.27112925988990	9.58473133974803
O	11.65144498141099	15.08745214880057	9.28126013175336
H	10.94350888595863	14.41482194258400	9.19877311977998
H	12.48022191805363	14.56914579288832	9.25811760618851
O	11.28880476734095	9.65935187781847	9.28396202990972
H	10.78868880571150	8.84407705575698	9.01654195153004
H	12.08656930758228	9.35031895708382	9.74452350628967

Surface charge=-2

1) Bare cluster

Energy=-8266.16277594738

H	5.77741510830110	18.48719919617974	2.80454894275873
H	5.77741499415044	13.04046337807160	2.76833022237233
H	5.77741498687516	7.59242012984517	2.73413664806733
H	13.48063509031453	13.03905259549357	2.77042346550206
H	6.55859727897839	3.22350855514496	5.83627545371896
Ga	5.80363070201084	19.12427817674776	5.98420128378039
Ga	5.77213826981292	13.67367778926270	5.98832482959315
Ga	5.80119004524284	8.12024212796058	6.04316864634685
Ga	13.46395274752281	13.68311106763813	6.03486745982254
H	12.70392628205083	8.66726177924078	5.87242505216877
H	1.92580493416041	13.03905177826662	2.77042464697098
H	9.62902517043612	18.48719932731128	2.80454882139182
H	9.62902504244577	13.04046307198372	2.76833076093021
H	9.62902483064005	7.59242105418224	2.73413534770136
H	0.77682476525852	11.44172607228531	3.92960752044927
H	14.62961387092532	11.44172603290528	3.92960799331148
Ga	7.70327835375618	16.35146008886216	3.87593954342352
Ga	7.70327519363692	10.90812212542978	3.85466136464791
Ga	7.70312772125606	5.31852885898761	3.94440974833032
Ga	7.70322070869414	21.84359771517444	3.88715233711005
Ga	3.82852247397405	16.35827895575198	3.87292515898223
Ga	3.83427289093905	10.87426106930929	3.86698712224376
H	4.62962017481163	5.99564048624797	3.89357732284106
Ga	11.57790979924991	16.35815406712615	3.87308113706862
Ga	11.57247280587624	10.87451819852978	3.86675333544768
H	10.77682057588854	5.99563916971104	3.89357708671946
Ga	1.94278871343965	13.68338091767934	6.03424784397068
H	2.70251344399315	8.66726134316112	5.87242543186579
H	8.84784145612282	3.22350887660862	5.83627573355523
Ga	9.60280154657298	19.12422924667094	5.98423012573784
Ga	9.63427497924491	13.67354253397090	5.98846094623269
Ga	9.60522942214181	8.12040323926110	6.04307799193994
H	0.74840069785034	11.67346251106455	7.64098898144516
H	14.65803969801662	11.67346264173050	7.64098962629521
Ga	7.70325825094338	16.66881493654687	7.53197321226829
Ga	7.70307073712458	11.18107970780556	7.46558659052277

Ga	7.70328594426559	5.17398478018327	8.51897068579929
Ga	7.70323465992868	22.19177714545174	7.44499665038447
Ga	3.91172875791842	16.73488211286827	7.49237110909652
Ga	3.76483004368102	11.18586664536418	7.52601357362019
H	4.60139081412274	6.22734723861122	7.60533346245693
Ga	11.49493174956898	16.73454305334307	7.49215819898113
Ga	11.64183022075432	11.18568540703586	7.52606565810863
H	10.80504974326465	6.22734635836117	7.60533300671246
P	5.78551854831244	17.72121785650252	4.00429621676664
P	5.76138963867434	12.29581477817120	3.98291337010558
P	5.78971586882789	6.82710225093518	3.94933180442423
H	6.38704562471043	22.71684345849397	4.00420320640884
H	12.85194065428474	17.25642358220869	3.96807755841539
P	13.48086522955415	12.28834537359272	3.98665291240441
P	5.81481520456809	17.88424993709519	8.10533674745947
P	5.74777793019928	12.36080243007876	8.01803073382418
P	5.76948397422371	6.94304556569445	8.02032919774988
H	6.39778609356491	22.90385779723418	7.89512872649508
H	12.85064291098239	17.45114195497497	7.85597212248770
P	13.54147554821227	12.43975168717345	8.08414155844737
H	7.70321980864698	4.53002827736785	2.61196078836058
H	7.70322000323181	20.84237176140982	2.68056191563790
H	7.70322004197820	15.40326649211452	2.65531099729418
H	7.70321992075975	9.95986312167589	2.62421714085885
H	3.85161006039172	15.39798399927803	2.64793621872327
H	3.85160996092074	9.96381130412405	2.62972783608873
H	11.55483002861323	15.39798439285244	2.64793743743516
H	11.55482990670750	9.96381191241806	2.62972868133714
H	2.55450149142792	17.25642178804092	3.96807763318214
P	1.92571718375585	12.28816451777903	3.98652493797030
P	9.62099046067727	17.72122904114311	4.00429078695846
P	9.64513595570145	12.29577994744068	3.98291885473385
P	9.61666339199916	6.82699808001901	3.94926099371137
H	9.01939437680667	22.71684270618605	4.00420262625839
H	0.63926639913514	14.47657188185647	5.89317721240246
H	14.76717414957146	14.47657321032997	5.89317633899078
P	7.70318940288162	4.09871961879144	6.00798572837289
P	7.70323036064346	20.48122851650040	5.90290375483248
P	7.70326494211642	15.01489554354832	5.88802911816625
P	7.70316351218686	9.53376075774310	5.81361705700395
H	4.48384897262509	19.92840929137666	5.92900072689648
P	3.87126456868145	15.03004775171977	5.89435937283044
P	3.83731660188637	9.52027499805576	5.85965727268906
H	10.92259266933855	19.92841061815801	5.92900143077454
P	11.53535360648200	15.02967880061802	5.89446795986317
P	11.56918293276976	9.52030711113415	5.85931572598896
H	2.55579675607711	17.45114105792187	7.85597164654626
P	1.86500417099854	12.43992134537769	8.08369388380880
P	9.59180612626477	17.88403378399980	8.10523109703252

P	9.65861416960894	12.36023920040786	8.01817363059277
P	9.63680684737233	6.94294997581029	8.02000848904619
H	9.00865282360101	22.90385821301087	7.89512904387055

2) Adsorbed H₁⁺*

Energy=-8266.63206181

H	5.77741503807760	18.48719918916805	2.80454892929134
H	5.77741498751128	13.04046338114797	2.76833019824331
H	5.77741485411337	7.59241997796958	2.73413663149565
H	13.48063511263967	13.03905255931378	2.77042348886523
H	6.55859727133593	3.22350866500201	5.83627550699807
Ga	5.80484169126893	19.12339613201190	5.97932617501720
Ga	5.79417820449705	13.64622218147502	5.94482051133471
Ga	5.84726802205437	8.29059965040669	5.98885918789598
Ga	13.45611579663712	13.69669099161201	6.04272538896408
H	12.70392630393953	8.66726168734800	5.87242505127275
H	1.92580479738442	13.03905170285360	2.77042466646184
H	9.62902520884181	18.48719932813102	2.80454882036133
H	9.62902501687160	13.04046306971275	2.76833073673743
H	9.62902482718071	7.59242089952965	2.73413550422696
H	0.77682488672509	11.44172617116535	3.92960748190032
H	14.62961382673212	11.44172606821837	3.92960798365401
Ga	7.71195129444051	16.33848505579384	3.88818525238634
Ga	7.72913678814003	10.86751756258589	3.90284079455750
Ga	7.70624029823984	5.43324183362831	3.84532423403964
Ga	7.70328091803052	21.84281007641671	3.88824018691752
Ga	3.82999025868691	16.35662953576077	3.87705541087624
Ga	3.83691980593264	10.88859006629135	3.85586307087964
H	4.62962025389535	5.99564060008481	3.89357725252994
Ga	11.58126644488670	16.34448105425268	3.88636779862569
Ga	11.56427525728130	10.88128323132479	3.87254193737247
H	10.77682053306151	5.99563924365065	3.89357697915584
Ga	1.94697413347505	13.69776764912250	6.02986726816706
H	2.70251340239171	8.66726132053046	5.87242541312239
H	8.84784151394782	3.22350875617287	5.83627569186903
Ga	9.60561919557446	19.11855096917230	5.98312531242663
Ga	9.61008956190847	13.58571126005835	6.05820926701439
Ga	9.59053089062735	8.30709715389765	5.98694544046159
H	0.74840055894350	11.67346246694635	7.64098895918335
H	14.65803969558462	11.67346264062855	7.64098962696736
Ga	7.70781635293531	16.66132794660207	7.52345891390495
Ga	7.93297709374010	10.44578175761847	8.56867642052542
Ga	7.70665715424221	5.79515312303357	7.56688975577093
Ga	7.70326461498668	22.19063811895569	7.44441782182977
Ga	3.91334366096676	16.73877554226068	7.48570621435044
Ga	3.68494132665778	11.21724381472314	7.55008234729677
H	4.60139097157990	6.22734727773681	7.60533347087122
Ga	11.50145888969630	16.71597745605731	7.47774966490686
Ga	11.63783293046018	11.28506921948589	7.61379024524402

H	10.80504957104724	6.22734641316138	7.60533300935261
P	5.79076244959855	17.71639842621278	4.00328934497407
P	5.77824227503328	12.27446587204668	3.96689919883891
P	5.76561865296533	6.86083700107036	3.96490486819867
H	6.38704560715501	22.71684295523573	4.00420293423772
H	12.85194061435366	17.25642352814127	3.96807749833554
P	13.48123603956883	12.29021354061436	3.99045288980063
P	5.81891951566100	17.88038251446577	8.10425227816956
P	5.80862220336414	12.16103748156960	7.84246373277665
P	5.72430729398489	7.01408231727380	8.00888288192350
H	6.39778622502542	22.90385793909195	7.89512866616726
H	12.85064295106686	17.45114196685547	7.85597214974605
P	13.58647957246112	12.47350854337984	8.10796278806347
H	7.70321988406553	4.53002839969464	2.61196078072865
H	7.70322006045796	20.84237209596806	2.68056227180488
H	7.70322004587555	15.40326647476452	2.65531094916074
H	7.70321992910158	9.95986313905791	2.62421718099232
H	3.85161002294730	15.39798408617660	2.64793628508315
H	3.85160996108725	9.96381137419100	2.62972791399670
H	11.55483004396685	15.39798445632516	2.64793748604811
H	11.55482991820769	9.96381193818694	2.62972867264574
H	2.55450154509648	17.25642173910432	3.96807754532763
P	1.92366588650158	12.29061612364587	3.98837798840310
P	9.62503974425200	17.71790053014866	4.00327078860574
P	9.64161114136989	12.29615002023066	3.98567535754297
P	9.64337054961787	6.86469404758634	3.96728837617496
H	9.01939433766180	22.71684285501495	4.00420263803212
H	0.63926663513686	14.47657179789895	5.89317725257743
H	14.76717414358417	14.47657321389258	5.89317633435960
P	7.70343628733401	4.07191612539254	5.86854779966768
P	7.70560904715783	20.47927714588411	5.90336765398268
P	7.71353303837051	14.99601195784579	5.89498867651513
P	7.70736459316272	9.71429249965468	5.97140551371318
H	4.48384893304235	19.92840938537047	5.92900079207021
P	3.88681042547916	15.01939330850455	5.89955681626765
P	3.81014847648952	9.55124845425306	5.87697356392440
H	10.92259256682448	19.92841055799317	5.92900137386484
P	11.50698372719167	15.00565642461275	5.89138690376359
P	11.60968078670608	9.57625861838939	5.91282126617269
H	2.55579677051448	17.45114106259011	7.85597163730461
P	1.82184075599236	12.47709404052971	8.10528298225453
P	9.59841672351345	17.87471312934687	8.09858273427561
P	9.64927514486964	12.35305773933664	8.07163509514169
P	9.68408191207414	7.01791637021047	8.00554473500981
H	9.00865278500640	22.90385803341398	7.89512904007219
H	5.40660102798580	13.12869111189927	8.80112398154564

3) Co-adsorbed H_1^+ * and H_2^+ *
Energy=-8267.11173665748

H	5.77741514931892	18.48719925891653	2.80454891216317
H	5.77741499805530	13.04046334629259	2.76833022382393
H	5.77741495291837	7.59242009502095	2.73413659035368
H	13.48063508715659	13.03905258140734	2.77042346977182
H	6.55859775584615	3.22350850814123	5.83627543800474
Ga	5.80532389519645	19.12722568863050	5.97805102446043
Ga	5.78835363515796	13.64946809519282	5.94158496391554
Ga	5.83620082748474	8.27983712665599	5.98498162745273
Ga	13.46228296282861	13.69452403856271	6.02841103908470
H	12.70392626127962	8.66726176245381	5.87242507859622
H	1.92580493169559	13.03905174423330	2.77042466592298
H	9.62902514010493	18.48719937635010	2.80454879011375
H	9.62902504531055	13.04046304467159	2.76833076852343
H	9.62902486319265	7.59242102604602	2.73413533082080
H	0.77682477219959	11.44172609096873	3.92960749354308
H	14.62961388160400	11.44172603099944	3.92960797623987
Ga	7.70321463552436	16.35147733185968	3.87672672587238
Ga	7.70327945083583	10.85934218754703	3.90592036595359
Ga	7.70296169726320	5.42585310350255	3.84753648826478
Ga	7.70322600022568	21.84564514523414	3.88496714408127
Ga	3.82727448882885	16.35609281518673	3.87479625544888
Ga	3.82704658795570	10.88662477670189	3.85473626932379
H	4.62962022310250	5.99564050199401	3.89357735415621
Ga	11.57912792265657	16.35603309399250	3.87478358111336
Ga	11.57949110123348	10.88652854283656	3.85471855046458
H	10.77682056003641	5.99563916913660	3.89357712132704
Ga	1.94426094964489	13.69468541370308	6.02862349075587
H	2.70251341669397	8.66726132288120	5.87242543837996
H	8.84784098552636	3.22350892062363	5.83627572901488
Ga	9.60122167149286	19.12705262980591	5.97802738736793
Ga	9.61805548114533	13.64948350362288	5.94157509968274
Ga	9.57018869021179	8.27983933774774	5.98512267229206
H	0.74840069926107	11.67346250553832	7.64098896178667
H	14.65803971866775	11.67346262817160	7.64098960742257
Ga	7.70317015508605	16.67813455852530	7.52954331317116
Ga	7.70310384940719	10.32460588703988	8.68792881146377
Ga	7.70328103646783	5.78228190183598	7.57093846119539
Ga	7.70331215857678	22.19341747705559	7.44578904207963
Ga	3.91221650769358	16.73947157313248	7.48967063082117
Ga	3.66585328126136	11.21120114654610	7.55238685853266
H	4.60139091774724	6.22734726938223	7.60533348297418
Ga	11.49427965545354	16.73886916603611	7.48967778259591
Ga	11.74040299769807	11.21159550852850	7.55214242496917
H	10.80504968087667	6.22734634864094	7.60533302788155
P	5.78504576699666	17.72028680387380	4.00363130882494
P	5.77005529258105	12.27652419928936	3.96830328586594
P	5.76729232620639	6.85899914040424	3.96255262162192
H	6.38704584651937	22.71684337981489	4.00420319997300
H	12.85194066827014	17.25642359702677	3.96807757702001

P	13.48462842266461	12.29193659823224	3.98842199597802
P	5.81415564379668	17.88520465258063	8.10526012844939
P	5.78771904745349	12.16375139703871	7.84248989473136
P	5.72713348038287	7.01196221758049	8.00746407955324
H	6.39778616578290	22.90385774263511	7.89512873397106
H	12.85064291847161	17.45114197863976	7.85597211877924
P	13.58982914851647	12.48146550489292	8.10842753806179
H	7.70321977268085	4.53002834945363	2.61196076673971
H	7.70321998710125	20.84237183604960	2.68056200132617
H	7.70322003134222	15.40326640615924	2.65531102140030
H	7.70321992596752	9.95986313552332	2.62421712511500
H	3.85161007645164	15.39798395039544	2.64793619028466
H	3.85160995607012	9.96381132309030	2.62972782339994
H	11.55483002615420	15.39798435050105	2.64793739313753
H	11.55482990212321	9.96381192665293	2.62972866965109
H	2.55450146390508	17.25642181025951	3.96807763917867
P	1.92178071573758	12.29203816283119	3.98835305710110
P	9.62134687130921	17.72022924898229	4.00354019292864
P	9.63645453179902	12.27654306605050	3.96826222408403
P	9.63894347228835	6.85887102116618	3.96250808019019
H	9.01939421006981	22.71684265040398	4.00420257702536
H	0.63926640649133	14.47657187516823	5.89317725914596
H	14.76717410933453	14.47657320730426	5.89317638170190
P	7.70321618892897	4.07023988682368	5.86920939737475
P	7.70334418415709	20.48238651870631	5.90539665688801
P	7.70320431053067	15.00971737005359	5.89591236449527
P	7.70322079627618	9.71079069554534	5.98797222230068
H	4.48384881264436	19.92840936417872	5.92900077225821
P	3.88528056860764	15.01983908817325	5.90245621109864
P	3.80861679312134	9.55263941400209	5.87717668255609
H	10.92259279216477	19.92841069332291	5.92900145184343
P	11.52118345060174	15.01964436614330	5.90223384816004
P	11.59781725106486	9.55262690614333	5.87720448408071
H	2.55579676079872	17.45114107574917	7.85597163636869
P	1.81640095377290	12.48119884975954	8.10843424502614
P	9.59242661829132	17.88500674315243	8.10507338990677
P	9.61859817409889	12.16398901622067	7.84270256463593
P	9.67945237349626	7.01185374923882	8.00748714015403
H	9.00865272846109	22.90385822265721	7.89512902714214
H	5.39678536796896	13.11860824129963	8.81579452943001
H	10.00950392330941	13.11876652470629	8.81607387047767

4) Adsorbed H₂⁺*

Energy=-8266.63213138827

H	5.77741506631867	18.48719923399458	2.80454895710501
H	5.77741498511237	13.04046333397173	2.76833024721745
H	5.77741492253071	7.59242008441840	2.73413659170183
H	13.48063516323046	13.03905252478736	2.77042349405866
H	6.55859767412344	3.22350855218635	5.83627545021705

Ga	5.80090603760888	19.11867456656920	5.98292330243371
Ga	5.79622522783949	13.58595362390570	6.05833647746642
Ga	5.81575922355877	8.30706891977849	5.98701468612915
Ga	13.45994245604459	13.69708232746279	6.02957206326688
H	12.70392625697790	8.66726177806441	5.87242509145238
H	1.92580492436670	13.03905172183196	2.77042470391582
H	9.62902523186491	18.48719935981265	2.80454882600766
H	9.62902505598644	13.04046304360278	2.76833076603047
H	9.62902486629611	7.59242100701935	2.73413533856208
H	0.77682479132230	11.44172611487255	3.92960749091941
H	14.62961380976915	11.44172610466599	3.92960795934377
Ga	7.69473504301677	16.33852060889167	3.88814451250100
Ga	7.67707957363902	10.86761040519792	3.90285665415922
Ga	7.69965400455315	5.43327326570382	3.84530564827904
Ga	7.70311935318626	21.84287956609361	3.88815558300109
Ga	3.82520399314859	16.34463342927337	3.88624690395160
Ga	3.84191237667724	10.88149249032872	3.87232049897564
H	4.62962023720258	5.99564051948788	3.89357735203857
Ga	11.57648749287116	16.35640806163214	3.87728967542783
Ga	11.56937642000580	10.88845702363742	3.85607027630177
H	10.77682054052498	5.99563918088611	3.89357711095486
Ga	1.95078154653077	13.69733420967591	6.04328075746966
H	2.70251343204757	8.66726130148645	5.87242540605167
H	8.84784107581130	3.22350888414942	5.83627572846980
Ga	9.60157242202529	19.12341821029941	5.97933527272797
Ga	9.61221882555819	13.64621304801178	5.94485317963915
Ga	9.55895444494898	8.29069636252765	5.98883561882489
H	0.74840072689453	11.67346250828893	7.64098898340860
H	14.65803976556375	11.67346260878757	7.64098959974777
Ga	7.69871094482906	16.66136151618538	7.52330229268039
Ga	7.47257481391824	10.44591648898793	8.56889139622367
Ga	7.69946517552646	5.79511792127126	7.56675453478316
Ga	7.70319872530532	22.19080187420644	7.44425587182501
Ga	3.90549750715405	16.71664207354154	7.47827709501845
Ga	3.76866213041091	11.28475864990398	7.61321366362729
H	4.60139085993600	6.22734724039935	7.60533348048978
Ga	11.49350150182824	16.73820792521675	7.48537803301208
Ga	11.72133831164080	11.21738519163207	7.55014337576989
H	10.80504971624124	6.22734634428940	7.60533302182781
P	5.78152310763195	17.71788268446426	4.00324209980124
P	5.76469329653656	12.29623553660978	3.98574923756004
P	5.76302367529253	6.86493136607388	3.96743547333808
H	6.38704560069565	22.71684343933908	4.00420323010171
H	12.85194062782585	17.25642355297675	3.96807747773874
P	13.48265453312065	12.29049490761038	3.98830258204280
P	5.80845099760398	17.87536460351530	8.09868211998384
P	5.75688875774305	12.35354512262752	8.07171373781786
P	5.72211638308191	7.01816846774750	8.00567848869317
H	6.39778605531256	22.90385779829242	7.89512871872143

H	12.85064294335854	17.45114197500840	7.85597211712547
P	13.58465711150997	12.47708161937093	8.10531303432377
H	7.70321979536064	4.53002837273005	2.61196078903971
H	7.70322003459104	20.84237179153162	2.68056197027415
H	7.70322003819130	15.40326641617039	2.65531093879975
H	7.70321994244604	9.95986313814686	2.62421711925207
H	3.85161009665188	15.39798397558243	2.64793626022540
H	3.85160993924041	9.96381133422438	2.62972782496239
H	11.55483003963155	15.39798444372562	2.64793750610453
H	11.55482989377717	9.96381194315242	2.62972866284399
H	2.55450143857901	17.25642182864548	3.96807759319102
P	1.92508504934817	12.29042428016347	3.99062542077045
P	9.61583102762857	17.71643902926655	4.00334322763040
P	9.62812317642332	12.27445016133625	3.96694505491792
P	9.64069697606886	6.86063708495273	3.96479244279746
H	9.01939439160133	22.71684269504145	4.00420259334835
H	0.63926638422876	14.47657189414576	5.89317720276773
H	14.76717406724295	14.47657319410750	5.89317637567071
P	7.70295054962080	4.07190174941537	5.86854951353226
P	7.70089264316654	20.47935750484114	5.90331622586023
P	7.69291602462435	14.99613488958293	5.89486356309461
P	7.69880456428068	9.71432749108394	5.97143857910180
H	4.48384900093461	19.92840926197432	5.92900073840088
P	3.89973859912763	15.00624443103523	5.89141863051839
P	3.79673543208581	9.57636287374909	5.91264860412034
H	10.92259265104063	19.92841062444150	5.92900141962849
P	11.52001920029287	15.01890039966734	5.89958795243628
P	11.59612050393685	9.55110143941720	5.87696654205434
H	2.55579671252836	17.45114108677735	7.85597165051261
P	1.82021373625878	12.47335610780439	8.10784800522751
P	9.58785049610024	17.87993400036197	8.10412533510288
P	9.59765738461959	12.16107426106758	7.84257602353490
P	9.68181277391731	7.01392491232174	8.00870269403299
H	9.00865285133130	22.90385820971454	7.89512903276119
H	10.00005605182562	13.12918568907512	8.80064709608359

5) Bare cluster + 1H₂O-OH*

Energy=-8418.55246148213

H	5.77741507832838	18.48719918804860	2.80454893184399
H	5.77741489992982	13.04046332643571	2.76833023865465
H	5.77741493321755	7.59242005668720	2.73413665578900
H	13.48063524426311	13.03905249247649	2.77042349124520
H	6.55859730835710	3.22350849110886	5.83627541846769
Ga	5.80123399350221	19.11554624702022	5.97978801250940
Ga	5.76359584769523	13.68610993882565	5.94849704758300
Ga	5.78049093856758	8.15559264391716	6.02792023074826
Ga	13.45717286057296	13.68320149185437	6.03483017845615
H	12.70392625021864	8.66726174685375	5.87242511300914
H	1.92580486668878	13.03905174527475	2.77042460369012

H	9.62902517170784	18.48719932097125	2.80454883654917
H	9.62902504891260	13.04046303262006	2.76833079652687
H	9.62902485298762	7.59242102613495	2.73413536742283
H	0.77682480606393	11.44172609244351	3.92960749112652
H	14.62961374598613	11.44172616268520	3.92960794948266
Ga	7.71525946389324	16.34983234283319	3.87733064221871
Ga	7.69332280134109	10.89730934350248	3.87170451911663
Ga	7.69836515729232	5.33763726305415	3.93771654891039
Ga	7.70326718821228	21.84073511822607	3.89039987987904
Ga	3.82454768501321	16.35597085745606	3.87450715426031
Ga	3.84087272386387	10.84596496223083	3.90492933833908
H	4.62962026420396	5.99564054754434	3.89357729585494
Ga	11.57717931828340	16.34407535254157	3.88810730031226
Ga	11.55415855354496	10.86884577398265	3.87746179930243
H	10.77682052712651	5.99563920987994	3.89357707664105
Ga	1.94506490321527	13.65532553182260	6.06208445236886
H	2.70251348484247	8.66726142648164	5.87242545169225
H	8.84784140646242	3.22350888736216	5.83627573793292
Ga	9.60424147155021	19.11810452205383	5.98584623730686
Ga	9.59587875351235	13.62276123545705	6.03441868646511
Ga	9.56174526368819	8.14684527185613	6.05550932522924
H	0.74840064518365	11.67346247468543	7.64098896618208
H	14.65803977373735	11.67346263325041	7.64098960167695
Ga	7.69812142539979	16.65803300149504	7.51499644468665
Ga	7.56583654055984	11.08534674362703	7.67126784166825
Ga	7.72190306598085	5.09696717585259	8.45289256560408
Ga	7.70312673308558	22.18838522359752	7.44395946198760
Ga	3.90654625080736	16.72124498181924	7.47195933152233
Ga	3.84487734471157	11.06942931485513	7.80432728209350
H	4.60139097049326	6.22734727407237	7.60533349018788
Ga	11.49539149417186	16.72113293426256	7.48854927515627
Ga	11.61533454767019	11.18418012516221	7.54660357367323
H	10.80504964707812	6.22734636810377	7.60533302362253
P	5.78791194253435	17.71552723967488	4.00017887556616
P	5.75712650930067	12.29136141865733	3.97482712303666
P	5.78528518351249	6.83644769130044	3.95171185352224
H	6.38704561680093	22.71684346173206	4.00420321444209
H	12.85194065917328	17.25642361703913	3.96807757099427
P	13.47481301421094	12.28307380835705	3.98633854273588
P	5.80955090772008	17.87425760980717	8.09990011714225
P	5.72859866556754	12.52131067332273	7.94983354331756
P	5.85399931235473	6.83181933556421	7.92378345740162
H	6.39778613069519	22.90385780940854	7.89512871836328
H	12.85064296552644	17.45114199261423	7.85597213913623
P	13.53553365304612	12.43470486430335	8.08159297350439
H	7.70321980594400	4.53002833439607	2.61196079947202
H	7.70322003729716	20.84237178263232	2.68056193939742
H	7.70322006368409	15.40326650917250	2.65531100456224
H	7.70321995274368	9.95986306620727	2.62421703018138

H	3.85161005505982	15.39798403113344	2.64793624545359
H	3.85160998567969	9.96381135517680	2.62972784537274
H	11.55483003694013	15.39798434867276	2.64793739320773
H	11.55482988996238	9.96381198501032	2.62972868902316
H	2.55450150995645	17.25642177037872	3.96807760881230
P	1.93251524664191	12.28286032494787	3.98832043527655
P	9.62620220139804	17.72170034455876	4.00269385782185
P	9.63511168771802	12.29239911458173	3.98551598016519
P	9.61734731572163	6.83509504736895	3.95515682201194
H	9.01939435220746	22.71684268912046	4.00420261120011
H	0.63926654891250	14.47657186930735	5.89317727495050
H	14.76717396731059	14.47657311538454	5.89317634956681
P	7.70612093491539	4.09772880029782	5.98974736187774
P	7.70245671785091	20.47619736550405	5.90413249984780
P	7.70458600664540	15.01893859560014	5.86661692284958
P	7.67855686266484	9.57879710386771	5.83793571605703
H	4.48384900834055	19.92840927222285	5.92900073123073
P	3.85492244977642	15.03564681913640	5.86837863669529
P	3.82398671741574	9.55426047374662	5.91471366184777
H	10.92259262791146	19.92841059562952	5.92900143494485
P	11.51016773039124	15.00169975491078	5.90552742164902
P	11.56102654279911	9.51410034112160	5.87250131215081
H	2.55579671337288	17.45114108171787	7.85597164709442
P	1.88300500271574	12.42038043769773	8.07805202533699
P	9.58979920625256	17.87327246783609	8.10299181406131
P	9.61169787190579	12.29963939027463	8.05415230249101
P	9.61318219241452	6.91387471296357	8.00739783290121
H	9.00865278513342	22.90385820619557	7.89512904127827
O	4.32504736258955	9.89381125719276	9.28598619351665
O	6.90775003929669	9.74387823558339	9.17660098495023
H	4.14556775076964	10.37647659981460	10.10920723590008
H	5.86968648503432	9.81635171460346	9.24394944153196
H	7.02695830979190	8.79498961669237	8.97061682561328

6) Adsorbed $H_1^+ + 1H_2O-OH^*$

Energy=-8419.02603745711

H	5.77741509976182	18.48719917719377	2.80454893637823
H	5.77741495143398	13.04046338373977	2.76833020140967
H	5.77741498744965	7.59242009512048	2.73413666531195
H	13.48063515883066	13.03905254355070	2.77042347504531
H	6.55859727147263	3.22350846272433	5.83627540526931
Ga	5.80448635953960	19.12507178950474	5.97705454303799
Ga	5.77731816732429	13.76989594990208	5.81548165178294
Ga	5.78493506818467	8.13245895065446	6.02592252885124
Ga	13.46053505890865	13.68188244898967	6.03699346587408
H	12.70392628260800	8.66726175824746	5.87242508454852
H	1.92580495811512	13.03905181910908	2.77042457718261
H	9.62902518757690	18.48719930481876	2.80454880974669
H	9.62902506441342	13.04046304078906	2.76833080094874

H	9.62902484995708	7.59242103533941	2.73413537973823
H	0.77682474437170	11.44172602830729	3.92960753437887
H	14.62961383463388	11.44172608771832	3.92960796445669
Ga	7.72517010078650	16.36598223439958	3.86389125757505
Ga	7.71784981780158	10.89841748290950	3.86641082742672
Ga	7.69952226334153	5.32720852151797	3.94091408674549
Ga	7.70335349721395	21.84439554480246	3.88604147104519
Ga	3.82435455766702	16.36685105855007	3.86387708134068
Ga	3.82299391705270	10.84431473741570	3.90247864063739
H	4.62962020060165	5.99564049837849	3.89357729801714
Ga	11.58029042188751	16.34410035653507	3.88553076179888
Ga	11.57017466209305	10.86744367208436	3.87503709052973
H	10.77682055131842	5.99563918881437	3.89357705938986
Ga	1.93908947183643	13.65032068653206	6.04847375965381
H	2.70251338133819	8.66726130560307	5.87242544554511
H	8.84784142088163	3.22350890904397	5.83627573662290
Ga	9.60416034251413	19.12500749397621	5.98694831440930
Ga	9.60734633345736	13.61509035615330	6.03406568662347
Ga	9.58382300527615	8.12145244033914	6.04072772409191
H	0.74840064819816	11.67346249566130	7.64098895936394
H	14.65803976465627	11.67346262810943	7.64098960658813
Ga	7.70528217434934	16.68036226153495	7.52712944409580
Ga	7.71841374630517	10.97142940834423	7.69849330411999
Ga	7.73092732393806	5.09854531088352	8.46879113831391
Ga	7.70311157864811	22.19154119520184	7.44525760711147
Ga	3.91089184165418	16.74181393612734	7.47987249756535
Ga	3.70105044030379	10.97906542666173	7.84710012080527
H	4.60139106565270	6.22734733112981	7.60533348857676
Ga	11.49659203713873	16.72332620403208	7.49306748153338
Ga	11.64024930787784	11.17318659694173	7.55923393721803
H	10.80504959736560	6.22734638739719	7.60533303249567
P	5.79053916545004	17.71750350539205	4.00157840862247
P	5.76108990118732	12.27521541390419	3.95672699275216
P	5.78677978384821	6.83177456649979	3.94831415495414
H	6.38704575990576	22.71684342468084	4.00420318789979
H	12.85194060078251	17.25642354294799	3.96807753308414
P	13.47890581938987	12.28643690948562	3.98746608929172
P	5.81320667255354	17.88409218287052	8.10602023824357
P	5.73499654661568	12.29788119613078	7.64571188567161
P	5.84946954747659	6.83960287191674	7.93433272829575
H	6.39778587682813	22.90385778827526	7.89512876594051
H	12.85064300226863	17.45114200310437	7.85597215976629
P	13.54325524298546	12.43918522557683	8.08818812780896
H	7.70321980067103	4.53002830594972	2.61196078919075
H	7.70321995786819	20.84237179867008	2.68056192899085
H	7.70322005795804	15.40326651172724	2.65531097397519
H	7.70321993163510	9.95986306339527	2.62421706663109
H	3.85161006425694	15.39798400682251	2.64793621846389
H	3.85160996412522	9.96381136718768	2.62972788789068

H	11.55483006929415	15.39798442403382	2.64793744205370
H	11.55482988657801	9.96381198013112	2.62972870657908
H	2.55450149015121	17.25642179030648	3.96807762874956
P	1.92897342346692	12.28386848612048	3.98666794373638
P	9.63303205419437	17.72681935020782	4.00451918219236
P	9.64631777058066	12.29278287397962	3.98593900846570
P	9.61601429050265	6.82770506982900	3.94912901471014
H	9.01939431497945	22.71684267320354	4.00420261113975
H	0.63926645456796	14.47657186334963	5.89317726603316
H	14.76717402400186	14.47657315071413	5.89317634428055
P	7.70597927895713	4.09678653157277	5.99623804838896
P	7.70406589317418	20.48056070927653	5.90312555270470
P	7.73045951720529	15.03668871984809	5.87385512512408
P	7.69125315310003	9.55226056751379	5.82211444985449
H	4.48384895564049	19.92840930965398	5.92900072047800
P	3.84381706951738	15.04733735044421	5.87731978407650
P	3.82236689614163	9.54550636810138	5.92099205547729
H	10.92259260129344	19.92841058004509	5.92900142934965
P	11.51184568431196	15.00115074404871	5.91042125512640
P	11.56386811797781	9.51699022784650	5.87202071928166
H	2.55579677657171	17.45114106160330	7.85597163173675
P	1.86027990976611	12.44396227720763	8.08866723938557
P	9.59684901317894	17.88371443957637	8.10714402009973
P	9.63875687820834	12.30947636489992	8.07839574407095
P	9.62097695919597	6.92496098500061	8.01237364823428
H	9.00865301784251	22.90385828025812	7.89512907303485
O	4.34032261801198	9.99639621569106	9.38185521676611
O	6.91639054656028	9.74503676996488	9.20420033369906
H	5.77023021144497	13.13575209993367	8.77871968011871
H	4.13453163636403	10.49897559816046	10.18602054770189
H	5.89302539525375	9.89307916150484	9.30938878362919
H	6.94850825196649	8.78417405857549	9.00433588820619

7) Bare cluster + 2H₂O-OH*

Energy=-8570.92972385919

H	5.77741509441833	18.48719917239374	2.80454892095661
H	5.77741498232383	13.04046343741560	2.76833018974488
H	5.77741500299907	7.59242011098667	2.73413666813183
H	13.48063510303450	13.03905260077484	2.77042343730274
H	6.55859733372674	3.22350847092209	5.83627540591013
Ga	5.79832567459619	19.10597380047579	5.97294198223002
Ga	5.74891384667307	13.72306807652884	5.94696895613393
Ga	5.77552307607215	8.15887239952856	6.02620731860858
Ga	13.44938417558538	13.68974764852364	6.03114928400695
H	12.70392628004028	8.66726176429867	5.87242505851088
H	1.92580498421820	13.03905185920214	2.77042455254986
H	9.62902511338830	18.48719933134829	2.80454885777975
H	9.62902506877182	13.04046307579479	2.76833079749018
H	9.62902483891276	7.59242105659890	2.73413535675881

H	0.77682471983295	11.44172599522235	3.92960755897444
H	14.62961387546320	11.44172601961625	3.92960799637461
Ga	7.70542420635302	16.34322207236122	3.89738152025419
Ga	7.68647864940498	10.90752320685302	3.86690047423642
Ga	7.69690711631151	5.33952440737583	3.93732809203666
Ga	7.70872322253055	21.83511071823285	3.89784060652503
Ga	3.82689367092202	16.33521186300446	3.91631137980805
Ga	3.83873878027494	10.85981618927523	3.90196462147637
H	4.62962018744363	5.99564050029100	3.89357729676489
Ga	11.56503361082395	16.34838357026466	3.89420727999259
Ga	11.54142102248852	10.87563444902416	3.87659235126239
H	10.77682056027106	5.99563918036191	3.89357707916797
Ga	1.98795085349232	13.70900202910729	6.08771921059756
H	2.70251338260892	8.66726129260514	5.87242543976111
H	8.84784136155888	3.22350893976690	5.83627573942785
Ga	9.59611829277549	19.09130646611309	6.03635493140619
Ga	9.55523530296426	13.66014798789612	6.04332022616725
Ga	9.56847066920331	8.14030854370452	6.04907280962298
H	0.74840064930482	11.67346250121030	7.64098897636352
H	14.65803972873831	11.67346262692770	7.64098961676261
Ga	7.57557314157125	16.56910914767563	7.73379977630169
Ga	7.57329630769777	11.05533538463098	7.63119014258294
Ga	7.72623442660299	5.09557087444071	8.44788715943944
Ga	7.70271887546367	22.17910599467581	7.42891817484281
Ga	3.95381974012293	16.61304774139206	7.79666718057754
Ga	3.83132205628161	11.06655737567386	7.80843344155268
H	4.60139100934065	6.22734731266546	7.60533348530675
Ga	11.48339633033847	16.71277634201085	7.51162435479524
Ga	11.60347325848091	11.19647638954446	7.53743423808152
H	10.80504965103331	6.22734636597797	7.60533303174864
P	5.78278114576143	17.71580267237525	3.99727357825609
P	5.75382344583825	12.30218678010320	3.98137619918912
P	5.78389252429774	6.83669804412189	3.95244395282391
H	6.38704549525578	22.71684348290164	4.00420321439766
H	12.85194061782078	17.25642354397568	3.96807752360878
P	13.47268663632244	12.28194645371600	3.98603586754591
P	5.80803412729466	18.04359044435811	8.04647363336785
P	5.74466094173349	12.46428552961939	7.90200896895199
P	5.85888290347618	6.82490576407742	7.91521016949034
H	6.39778612532370	22.90385789938265	7.89512875010234
H	12.85064293868032	17.45114205640573	7.85597217082393
P	13.53295120703274	12.43488267593462	8.07691451846418
H	7.70321978392917	4.53002827932766	2.61196079338759
H	7.70322008477547	20.84237175094419	2.68056191831136
H	7.70322006894968	15.40326649397601	2.65531099430809
H	7.70321991695044	9.95986301947790	2.62421706836248
H	3.85161004875793	15.39798400611882	2.64793619755475
H	3.85160995710239	9.96381131881983	2.62972787064544
H	11.55483007854230	15.39798445365220	2.64793746040951

H	11.55482989457490	9.96381194690589	2.62972871764639
H	2.55450152195343	17.25642176919074	3.96807765589555
P	1.92824643295571	12.29617520138011	3.99951822641422
P	9.61879868860529	17.72494910131041	4.00986393340859
P	9.62756155492542	12.30435255564750	3.99375984327344
P	9.61787736374476	6.83220445230023	3.95361767665018
H	9.01939440500127	22.71684273138915	4.00420262710267
H	0.63926644548197	14.47657187012417	5.89317726153994
H	14.76717411350477	14.47657320859400	5.89317632865004
P	7.70650314002905	4.09807334556186	5.98906263522885
P	7.70868327093705	20.47789971532752	5.88466129864615
P	7.68142886838943	15.07134105397505	5.90100108411655
P	7.68629204032427	9.55481844269154	5.81202710845956
H	4.48384901950532	19.92840927193588	5.92900072598943
P	3.87290786767141	15.10590736341387	5.93324544410888
P	3.82012297955594	9.55834017901298	5.91222238956882
H	10.92259275055473	19.92841041638343	5.92900134509041
P	11.50326324882309	15.00098095804827	5.91133495570915
P	11.56086203334507	9.51550688897007	5.86987062180057
H	2.55579664337948	17.45114110387007	7.85597167425193
P	1.87801239769076	12.42664999589802	8.08556453537743
P	9.56258050181257	17.81809488513220	8.13599428418009
P	9.59524323177555	12.29485528614908	8.04673267580845
P	9.61490803056327	6.91615189319045	8.00805463301204
H	9.00865277980082	22.90385816909986	7.89512905712446
O	4.30931056547518	9.88451540273584	9.28577390668287
O	6.90914665072450	9.71902995879943	9.16010570999905
H	4.14322029186863	10.37345854434719	10.10798685304152
H	5.87839947675763	9.80788456515674	9.23249379478541
H	7.00142966858104	8.76826969956096	8.94446545104557
O	4.32406630684736	15.43564281365695	9.33026902861329
O	6.90796026798631	15.20609410624779	9.24177577673020
H	4.18775234242736	15.97623220275386	10.12536425751309
H	5.87161739092238	15.31326712361290	9.29983440224597
H	6.98052076512263	14.26527799111458	8.97217468928550

8) Adsorbed $H_1^+ + 2H_2O - OH^*$

Energy=-8571.40859677237

H	5.77741508417240	18.48719915070657	2.80454893122009
H	5.77741497459797	13.04046339324505	2.76833020446698
H	5.77741499453217	7.59242011146804	2.73413664632830
H	13.48063509094890	13.03905260075562	2.77042344394418
H	6.55859737089794	3.22350845180606	5.83627540232156
Ga	5.79484152896898	19.10820222267698	5.97477006521604
Ga	5.75342996887122	13.82235345557382	5.81596195729867
Ga	5.78126140564669	8.14036638240779	6.02736884624342
Ga	13.45196572979549	13.68989435374815	6.03266462609905
H	12.70392627430500	8.66726173046459	5.87242507457401
H	1.92580497904172	13.03905184312198	2.77042456298157

H	9.62902511333224	18.48719932003161	2.80454884136182
H	9.62902506056463	13.04046307035936	2.76833079486221
H	9.62902486174491	7.59242102563860	2.73413538407128
H	0.77682473007477	11.44172600844485	3.92960755397033
H	14.62961387983790	11.44172602031704	3.92960799040973
Ga	7.71685046141856	16.36132446361669	3.88042613920956
Ga	7.70517325939125	10.91107543346766	3.86112004061540
Ga	7.69880501638508	5.33009832029852	3.94035916723740
Ga	7.70809965394539	21.83674970528362	3.89598142090291
Ga	3.82591935920079	16.35200808678196	3.89585222320168
Ga	3.82112901704165	10.86227458097139	3.89552442024989
H	4.62962020169932	5.99564049955430	3.89357730582699
Ga	11.56794696386434	16.34914882720145	3.89089750856893
Ga	11.55776644477111	10.87430920695272	3.87462688808796
H	10.77682053194782	5.99563920223268	3.89357706136559
Ga	1.98249491566296	13.70471043615939	6.07112253549797
H	2.70251335633614	8.66726129595073	5.87242544299315
H	8.84784132343629	3.22350894484214	5.83627573223663
Ga	9.59578830252184	19.10131446720406	6.03461843504479
Ga	9.56124034949319	13.65941894887852	6.03149817858636
Ga	9.58337169656953	8.12807513023673	6.04065082831598
H	0.74840065400157	11.67346250111279	7.64098896965286
H	14.65803972907244	11.67346262209873	7.64098961163455
Ga	7.58989469971508	16.60003474295128	7.73868151725951
Ga	7.69981417400755	10.97950595350641	7.67954527608496
Ga	7.72904304766150	5.10611912597842	8.46531935224132
Ga	7.70265854395343	22.18106075627537	7.43089998727661
Ga	3.96293150480790	16.60707063171181	7.81148940133458
Ga	3.69383140704578	10.98461777163319	7.82389199271230
H	4.60139110989351	6.22734734359603	7.60533349740697
Ga	11.48360921562096	16.71861437862783	7.51412913775971
Ga	11.62310071361720	11.19242350447902	7.55595322693564
H	10.80504956884362	6.22734638166153	7.60533303775508
P	5.78573723600810	17.71762499238367	3.99724702309180
P	5.75634579325935	12.29192641308599	3.96666074979454
P	5.78592619707340	6.83338883970914	3.94984361969727
H	6.38704550072073	22.71684347754786	4.00420321437320
H	12.85194062187237	17.25642353228717	3.96807752286940
P	13.47683219154404	12.28547134194027	3.98716551887200
P	5.80273117782598	18.04544884245563	8.05352654227189
P	5.71616643579677	12.28948633229919	7.60778813755725
P	5.84677736591170	6.84470990462062	7.93571763112126
H	6.39778613617626	22.90385788884799	7.89512873943442
H	12.85064294355294	17.45114201955474	7.85597212834799
P	13.54093255646126	12.44210026046267	8.08390045213588
H	7.70321978916752	4.53002828237497	2.61196077196264
H	7.70322007956750	20.84237174586345	2.68056190798904
H	7.70322007926457	15.40326648996133	2.65531097835756
H	7.70321992213369	9.95986303829191	2.62421707250850

H	3.85161004335711	15.39798401652811	2.64793619107384
H	3.85160995685015	9.96381133996472	2.62972786014100
H	11.55483007409090	15.39798445008080	2.64793745603656
H	11.55482990478875	9.96381195122439	2.62972871361940
H	2.55450153235362	17.25642176407701	3.96807766109691
P	1.92370949697904	12.29767868167811	3.99778673815160
P	9.62608618508611	17.73112936625058	4.01097129995659
P	9.63749545678355	12.30295769936918	3.99247544561626
P	9.61663281191670	6.82903746751724	3.95009949724081
H	9.01939439425939	22.71684271551265	4.00420262702713
H	0.63926645206679	14.47657187258327	5.89317726606376
H	14.76717412058985	14.47657322260915	5.89317634950207
P	7.70585011427653	4.09742958332207	5.99523098316230
P	7.70514815327999	20.47853199614683	5.88652637475640
P	7.70456898745424	15.09612896567558	5.89954130140648
P	7.69033715106488	9.55253616898936	5.81345515571514
H	4.48384901913315	19.92840928850526	5.92900072045500
P	3.85156208513323	15.12610290493981	5.91923811168810
P	3.81819652261635	9.54684415527554	5.91049645145334
H	10.92259274905746	19.92841052114931	5.92900143008369
P	11.50384956480324	15.00175229295527	5.91569741404666
P	11.56348984212878	9.52164060128733	5.87323590959813
H	2.55579663462153	17.45114110332692	7.85597167935428
P	1.85701776209881	12.44887108561641	8.09395240471617
P	9.57090451047135	17.83692402771579	8.13471827129638
P	9.61273239418007	12.32449435796572	8.07456997675125
P	9.62004066538575	6.92625506327904	8.00914585621790
H	9.00865277436873	22.90385815857338	7.89512905718586
O	4.34047685645500	10.01329431155395	9.37284168383819
O	6.90865831256779	9.76371032136161	9.20314572553715
H	5.66668658369754	13.08903021695726	8.76417734734592
H	4.13148224098197	10.51847804622999	10.17473314002192
H	5.88003738152197	9.90699254627147	9.30020259201728
H	6.95117653813644	8.80141221473978	9.01536490061099
O	4.45241421900686	15.25455239363120	9.20079351738878
O	6.96032278213603	15.26530628591255	9.22877140408013
H	4.15092169675868	15.52590576804963	10.08159526630796
H	5.87833233947272	15.22623365663241	9.23851885066165
H	7.31910025834138	14.36526685216923	9.18836232343886

9) Bare cluster + 2H₂O-OH* +3H₂O*

Energy=-8800.22201826826

H	5.77741513430564	18.48719920864213	2.80454892474827
H	5.77741494122915	13.04046339239519	2.76833022515051
H	5.77741487956851	7.59242000867640	2.73413665864454
H	13.48063508297470	13.03905260514006	2.77042344678601
H	6.55859717329878	3.22350836698664	5.83627544699162
Ga	5.82536328471931	19.13535986889951	5.95063151780212
Ga	5.76229793520012	13.74024230291005	5.94790512964488

Ga	5.78796932629123	8.17541086540601	6.03385385333921
Ga	13.43266318644280	13.68358325676569	6.03723943574743
H	12.70392636614354	8.66726170501107	5.87242506010285
H	1.92580493466130	13.03905183588732	2.77042456610959
H	9.62902519638918	18.48719932239724	2.80454879838726
H	9.62902504944061	13.04046309322126	2.76833078135686
H	9.62902477884757	7.59242101409005	2.73413538263060
H	0.77682475900348	11.44172602833806	3.92960755569159
H	14.62961387848086	11.44172602365617	3.92960799397004
Ga	7.71129738810708	16.34512110850435	3.89954542241756
Ga	7.68944931305390	10.91061631807111	3.86934474966975
Ga	7.69055074522374	5.33811202893126	3.93879537080416
Ga	7.70989452907737	21.82209225075834	3.91839751576567
Ga	3.83102662793585	16.33994280300581	3.91522638536357
Ga	3.84193244005322	10.86408329305462	3.90122550667215
H	4.62962033241500	5.99564061839312	3.89357730905185
Ga	11.56685703104397	16.34439967639880	3.89948239521835
Ga	11.55005762798402	10.88573640186711	3.86950719323514
H	10.77682058109931	5.99563914934164	3.89357702944399
Ga	1.99224428978978	13.71521139298686	6.09164859262076
H	2.70251349764620	8.66726135225964	5.87242544803592
H	8.84784142332079	3.22350897564949	5.83627574802643
Ga	9.59954569604974	19.07384961035223	6.04124624235602
Ga	9.58647589296212	13.67016277930011	6.02796581303014
Ga	9.60542260356142	8.17451292420521	6.01284778843026
H	0.74840061813212	11.67346247412943	7.64098896614428
H	14.65803973861398	11.67346262079434	7.64098961484301
Ga	7.59380653412973	16.58805757580177	7.73911807131803
Ga	7.58588875475111	11.10272202048860	7.64920538478924
Ga	7.72131030441850	5.13861117218092	8.48824175143123
Ga	7.70457321654819	22.02864251421668	7.63780731352224
Ga	3.95562727750061	16.62443212709227	7.79975779218336
Ga	3.83661336142912	11.07091876051721	7.80538396995061
H	4.60139089988861	6.22734722254715	7.60533346566277
Ga	11.51185277341018	16.58529556212213	7.67489626556352
Ga	11.56286708098969	11.05867689395210	7.68996475337849
H	10.80504965547031	6.22734645049524	7.60533303327202
P	5.78525266697567	17.71661061571513	3.99672397680026
P	5.75607989579815	12.30775061911170	3.98491941264814
P	5.78327915034782	6.84086940598866	3.95633379198360
H	6.38704549455676	22.71684348303384	4.00420321986256
H	12.85194060269762	17.25642354182788	3.96807752829759
P	13.47591082765163	12.28647643668403	3.98628897616614
P	5.81534363962688	18.05911949071453	8.03087744348151
P	5.73662798542861	12.48267712417903	7.90527522919374
P	5.84507284062381	6.84691671422132	7.92857624871991
H	6.39778623630778	22.90385787350825	7.89512873451185
H	12.85064299766633	17.45114201062721	7.85597217412174
P	13.50113201473946	12.39969112587763	8.05751002880624

H	7.70321986587756	4.53002841105935	2.61196080081282
H	7.70322007453366	20.84237175052600	2.68056191815114
H	7.70322004711817	15.40326649654147	2.65531097705849
H	7.70321992889521	9.95986303838787	2.62421706108905
H	3.85161004631530	15.39798401881962	2.64793623168516
H	3.85160998968443	9.96381132308616	2.62972787907346
H	11.55483005858082	15.39798443664114	2.64793745115008
H	11.55482989328760	9.96381194415421	2.62972871371714
H	2.55450149017155	17.25642177510812	3.96807761620605
P	1.92850308962084	12.29770985053675	4.00057658018847
P	9.62532888331502	17.72220038386000	4.00747485793071
P	9.63009286565794	12.30423259915110	3.99130287433609
P	9.61472901095378	6.82891720964828	3.95163088010173
H	9.01939443215664	22.71684272615147	4.00420261646801
H	0.63926642218078	14.47657190379664	5.89317725515393
H	14.76717409668630	14.47657320311333	5.89317635605416
P	7.70749999460753	4.09975432275253	5.99684624736731
P	7.72953408208882	20.49721221439161	5.87890207340997
P	7.69711456195833	15.08148174295860	5.90639623731030
P	7.70102303082915	9.57769902370824	5.83151309020635
H	4.48384901303376	19.92840926727428	5.92900071934892
P	3.87872213104758	15.11569888678603	5.93652570658870
P	3.82097510300836	9.56005422762757	5.91141999607405
H	10.92259257430857	19.92841055765979	5.92900142997398
P	11.51171967429439	15.02942638726719	5.89339607065914
P	11.57982920682338	9.54655941332690	5.84498282768058
H	2.55579677408441	17.45114105104312	7.85597166294976
P	1.87882303754846	12.42573865677837	8.08602956031220
P	9.57918609708602	17.81816555210673	8.13326283352606
P	9.61243072618957	12.34407188865936	8.03378447314146
P	9.65896562204776	6.98315889016251	8.00667135676246
H	9.00865266878489	22.90385814232017	7.89512903083844
O	4.32535663234391	9.89587886379001	9.28709005485272
O	6.92893660686405	9.74755702022262	9.16962940296716
H	4.16483018908268	10.39106160832671	10.10672844923015
H	5.89596372328458	9.82001401723290	9.23182498780321
H	7.04698714617777	8.80001416117273	8.96040326145959
O	4.33580129406045	15.45568107645476	9.33478618505887
O	6.92224213636884	15.22468334582382	9.24554360220104
H	4.20942318546639	16.00327107036331	10.12679822022238
H	5.88658172242712	15.32506487292399	9.29867399577313
H	7.00824899628916	14.28475627950758	8.98013111104613
O	7.71385430497409	20.52078598025157	9.21510215438875
H	8.50392393415765	19.94539674807023	9.10532094460668
H	6.97247724762465	19.88716621387173	9.02881978868789
O	11.61113597415200	15.03945437899769	9.24286575002860
H	10.89861874855801	14.37769367335303	9.09701030848657
H	12.43348565903051	14.51206121046261	9.19393181122722
O	11.30871544953735	9.56079651984553	9.19628922410909

H	10.77263861486882	8.76394675545116	8.88446630006076
H	12.13526329672724	9.19699185162943	9.55446029960506

10) Adsorbed $H_1^+ + 2H_2O - OH^- + 3H_2O^*$

Energy=-8800.22201826826

H	5.77741512954272	18.48719920499088	2.80454892587661
H	5.77741494606220	13.04046338450045	2.76833023073422
H	5.77741489190423	7.59242003827765	2.73413663213055
H	13.48063508888020	13.03905259960955	2.77042345005883
H	6.55859725807101	3.22350835717036	5.83627543071167
Ga	5.82161930353839	19.13947787787639	5.95374441932224
Ga	5.76453804093830	13.83593911922848	5.81528344976056
Ga	5.79446235440541	8.15588084277119	6.03342706349804
Ga	13.43590051678957	13.68351024765498	6.03903944769364
H	12.70392634185166	8.66726171756459	5.87242505291043
H	1.92580494828270	13.03905182990365	2.77042457600632
H	9.62902520236704	18.48719931688584	2.80454880495497
H	9.62902505109241	13.04046308121156	2.76833079423280
H	9.62902478503549	7.59242103702227	2.73413537203373
H	0.77682474400141	11.44172602830936	3.92960754440433
H	14.62961387657479	11.44172602881955	3.92960799254750
Ga	7.72159851811319	16.36388511867841	3.88155240390879
Ga	7.70892289762822	10.91291840966592	3.86463671566345
Ga	7.69354195186209	5.32872032035486	3.94219055177149
Ga	7.70816405010960	21.82248577658667	3.91815890027526
Ga	3.83048623547436	16.35705682431762	3.89452391190355
Ga	3.82415440463200	10.86593346411989	3.89527729608826
H	4.62962031391714	5.99564059366595	3.89357730485786
Ga	11.56984363803401	16.34430214929356	3.89773519174395
Ga	11.56575491933429	10.88325628468833	3.86849531856746
H	10.77682058411026	5.99563914304792	3.89357702741331
Ga	1.98668543833895	13.71059521896402	6.07456482872489
H	2.70251350514288	8.66726135732164	5.87242543659176
H	8.84784135391990	3.22350897506670	5.83627572869721
Ga	9.59958457164048	19.08303397504074	6.03980948224582
Ga	9.59127624762987	13.66897856989090	6.01699958887240
Ga	9.62068926816587	8.16535319328960	6.00827581468388
H	0.74840064821402	11.67346249455744	7.64098896517847
H	14.65803972338873	11.67346263333532	7.64098961523580
Ga	7.60415489714002	16.61615205803394	7.73789296748199
Ga	7.70276800400905	11.02947969390601	7.70238848114013
Ga	7.72651597354438	5.14812209975912	8.50858496161689
Ga	7.70419306639319	22.03144650616016	7.64129861204258
Ga	3.96286546115982	16.61609424319478	7.81407462185413
Ga	3.69536794316974	10.98575860926334	7.82206454804882
H	4.60139097908878	6.22734725080729	7.60533348627864
Ga	11.51338165100645	16.59279129031983	7.67918581343299
Ga	11.58191958554487	11.05856329316101	7.71152396759028
H	10.80504957870811	6.22734646551458	7.60533305386220

P	5.78813558840161	17.71952416959569	3.99722422729835
P	5.75886551341237	12.29608343686884	3.96940571189164
P	5.78552281740668	6.83710729925387	3.95320728085758
H	6.38704549422505	22.71684348321778	4.00420321986362
H	12.85194059549917	17.25642353465159	3.96807752799961
P	13.47981081134709	12.28974331032943	3.98738002815534
P	5.80922829878396	18.05743245306677	8.03817671367094
P	5.70578503839830	12.30359246909188	7.60829508803670
P	5.83449535825964	6.86413598974211	7.94573539900374
H	6.39778624161800	22.90385787323217	7.89512873444152
H	12.85064299597936	17.45114200926391	7.85597217199562
P	13.50914567889255	12.40861071246888	8.06516719384240
H	7.70321984457783	4.53002839340696	2.61196082428169
H	7.70322007447354	20.84237175040877	2.68056191786352
H	7.70322004671610	15.40326649460705	2.65531097358078
H	7.70321992585998	9.95986303467532	2.62421706047641
H	3.85161003848121	15.39798403131645	2.64793623803377
H	3.85160998403232	9.96381132911944	2.62972788725293
H	11.55483006535075	15.39798443666496	2.64793745039650
H	11.55482989687498	9.96381194163734	2.62972871053936
H	2.55450151367344	17.25642176205494	3.96807761834441
P	1.92399428316094	12.29901991230924	3.99876887996058
P	9.63252597278891	17.72805040366463	4.00851591235326
P	9.64025285427418	12.30277238176342	3.99003261506388
P	9.61417212668543	6.82706107328837	3.94947054787229
H	9.01939443243937	22.71684272646027	4.00420261649321
H	0.63926640469936	14.47657189412653	5.89317726076158
H	14.76717408797801	14.47657318888922	5.89317635047121
P	7.70707096365893	4.09882432573306	6.00322834221354
P	7.72674056839061	20.49754243467565	5.88310905165150
P	7.71803478929225	15.10330383845229	5.90119717903142
P	7.70427901508067	9.57607669457651	5.83574195169803
H	4.48384900490409	19.92840927533492	5.92900072000454
P	3.85706656438841	15.13468817492481	5.92117115497545
P	3.81925732684205	9.54769245060678	5.91009682090573
H	10.92259255931505	19.92841054793069	5.92900143507765
P	11.51201842930886	15.02949514316114	5.90071448129159
P	11.58341770876085	9.55410487030175	5.85202034066113
H	2.55579679680155	17.45114104087959	7.85597165817446
P	1.85712548257702	12.44830601060779	8.09451943157110
P	9.58535755910331	17.83192581636574	8.13197338698382
P	9.62430527312532	12.37048323527112	8.05709075707193
P	9.66566003127593	6.99253971923971	8.00981034809469
H	9.00865266361942	22.90385814256287	7.89512903080470
O	4.34908864552855	10.02460591563178	9.37605108792987
O	6.92218626260560	9.78562325049253	9.21436804072789
H	5.64323210468750	13.10102070544053	8.76521588459731
H	4.13877752385706	10.53598082727945	10.17371921772646
H	5.89301593929055	9.92308467133299	9.30760432635468

H	6.97107160042990	8.82608277805377	9.01995987388014
O	4.44714886188412	15.27182463837688	9.20504770553762
O	6.96864619844860	15.26271661619838	9.22130350606181
H	4.17029720623363	15.57080565668643	10.08524431757712
H	5.89599131708402	15.23217523222672	9.23198899250570
H	7.31241810029701	14.35831167831460	9.15075269797505
O	7.71318304476424	20.53091626111955	9.22596196205108
H	8.50063511518237	19.95229110810254	9.11756894247190
H	6.96814123345379	19.90108661323030	9.05024250917688
O	11.64513339433235	15.08418146245621	9.27356457875745
H	10.92544919529367	14.42485920073466	9.18410095862382
H	12.46341772746704	14.55115690781867	9.22241005430988
O	11.28752541665023	9.58213904561437	9.21430727031385
H	10.77433375922636	8.77074913958219	8.89929331202165
H	12.09978219215404	9.24130737269434	9.62453290753865

11) Adsorbed $\text{H}_2^+ + 2\text{H}_2\text{O} - \text{OH}^+ + 3\text{H}_2\text{O}^+$

Energy=-8800.70180373492

H	5.77741509942225	18.48719919447821	2.80454894726902
H	5.77741490605536	13.04046333978362	2.76833024928834
H	5.77741492255236	7.59242009118557	2.73413665383460
H	13.48063510292235	13.03905259358419	2.77042344242872
H	6.55859737308300	3.22350849606617	5.83627544203703
Ga	5.84187718834985	19.20672823666264	5.80860421151952
Ga	5.76363147211429	13.70065444213789	5.94311916714132
Ga	5.78864683354357	8.17120300069296	6.03382543891818
Ga	13.43673724851640	13.68106851597348	6.04066894655255
H	12.70392628043131	8.66726174700826	5.87242508232386
H	1.92580497978905	13.03905185744825	2.77042453946328
H	9.62902517607107	18.48719931641595	2.80454879889426
H	9.62902505353560	13.04046305618374	2.76833077546311
H	9.62902482157435	7.59242105859412	2.73413537933932
H	0.77682470857184	11.44172598581896	3.92960756258371
H	14.62961387599332	11.44172602931375	3.92960798821784
Ga	7.73221041484688	16.34292862801742	3.89339912606707
Ga	7.69456258059135	10.90180152048046	3.87165981980515
Ga	7.69104362590115	5.33635622806875	3.93954352115448
Ga	7.71183483315950	21.83350253052300	3.90691161474728
Ga	3.81509339940083	16.33338515802860	3.91314463056180
Ga	3.84144932202757	10.85243114761154	3.90468388817747
H	4.62962026257519	5.99564054490677	3.89357730444443
Ga	11.57801656287482	16.33801552420847	3.89909144709262
Ga	11.56320351528107	10.87862922971243	3.86974492433524
H	10.77682056877980	5.99563917374442	3.89357706134098
Ga	1.96826459715409	13.67641656379658	6.07059817181147
H	2.70251349177933	8.66726139209281	5.87242544396061
H	8.84784132551096	3.22350893692254	5.83627573003504
Ga	9.61054376362292	19.05954623854777	6.03285514821224
Ga	9.61184884085599	13.63095927856510	6.01066411626014

Ga	9.60723351442549	8.17174744840805	6.01349310551538
H	0.74840068674042	11.67346249406173	7.64098896682343
H	14.65803970365992	11.67346264743407	7.64098961259117
Ga	7.72557498164957	16.44562900358636	7.74339820226467
Ga	7.59110141447227	11.09802698634879	7.65843667444417
Ga	7.72040493387952	5.13730468628456	8.49043970209330
Ga	7.71168442002777	22.05104313482282	7.63891492468162
Ga	3.83439643821608	16.48867908292996	7.81283803911235
Ga	3.83376940970654	11.06867134546351	7.81796149287970
H	4.60139082134910	6.22734721847351	7.60533344724188
Ga	11.52824768907309	16.57071987766624	7.69104961364904
Ga	11.57076947198428	11.05225850317763	7.69707701234410
H	10.80504974276982	6.22734634663244	7.60533299100869
P	5.78818295478062	17.69655700460544	3.97434800354795
P	5.75733122766842	12.29483742390059	3.97677931552222
P	5.78345594696409	6.84023921652734	3.95559575093532
H	6.38704551070502	22.71684347780759	4.00420321458044
H	12.85194059483015	17.25642353043019	3.96807754668644
P	13.47801695307185	12.28822008254052	3.98699482610352
P	5.81681900687227	17.80415149398245	7.70305530591834
P	5.74071256792101	12.48254803238929	7.91691172491075
P	5.84469818243362	6.84733073524188	7.93015544539464
H	6.39778625751472	22.90385785717212	7.89512872386480
H	12.85064302932228	17.45114201419822	7.85597217742241
P	13.50319739868047	12.40008470698122	8.06096240530350
H	7.70321981317070	4.53002832241233	2.61196086857467
H	7.70322007449584	20.84237176639948	2.68056193381993
H	7.70322005303994	15.40326649901729	2.65531099475385
H	7.70321994864451	9.95986305606545	2.62421701539390
H	3.85161007158535	15.39798398135460	2.64793619503075
H	3.85160998303776	9.96381131463978	2.62972783621968
H	11.55483007065230	15.39798441963983	2.64793743344895
H	11.55482989635554	9.96381196206939	2.62972870604559
H	2.55450148117428	17.25642179389093	3.96807764622919
P	1.93090398376073	12.28804470363813	3.99293234796101
P	9.63490041999748	17.71899359461711	4.00465278601856
P	9.63856107067547	12.28860149075820	3.98053216791871
P	9.61471348836046	6.82865809351072	3.95134680192997
H	9.01939441058847	22.71684271034254	4.00420261648297
H	0.63926645640926	14.47657188910207	5.89317727152953
H	14.76717408336108	14.47657317662840	5.89317634008196
P	7.70755214672295	4.09905552083647	5.99761460801650
P	7.75483794767224	20.50661640867600	5.88812842756267
P	7.71160548477457	15.02931546462408	5.87498919648666
P	7.70157572352386	9.57734438743855	5.83653799056835
H	4.48384903390304	19.92840924643080	5.92900073135431
P	3.86629969718645	15.06653859879260	5.91882636889225
P	3.82190953301736	9.55953696358761	5.91819761691452
H	10.92259267091613	19.92841061683776	5.92900142981098

P	11.51088586680681	15.02901529211937	5.89683083068550
P	11.58075777892074	9.54664673259333	5.84718445189097
H	2.55579663726878	17.45114110953655	7.85597167976824
P	1.87761101175661	12.42685952809895	8.08485317275730
P	9.58181939128733	17.81175542999500	8.14779682437956
P	9.61928220775240	12.34258600955209	8.03345009860470
P	9.66089055332684	6.98476272108119	8.00902671390818
H	9.00865265300798	22.90385814273183	7.89512903071936
O	4.32954967093043	9.89725469519305	9.29651128786840
O	6.93262201134915	9.74652660052352	9.17443789193309
H	4.16751408842440	10.38802526671782	10.11851146344744
H	5.89975075307831	9.81970382452212	9.24006125589320
H	7.04950639586546	8.79802730418746	8.96796802587628
H	5.87910499560092	18.63946892125358	8.83966473304288
O	4.34088726128726	15.50319207152524	9.40926223770530
O	6.93077169451165	15.20114879991811	9.26562176581592
H	4.18948116584119	16.08570412649046	10.17092070347436
H	5.90791736142966	15.35725500881336	9.34767684103945
H	6.94904682060618	14.24799075984771	9.01946556457360
O	7.92959130313629	20.64221947932779	9.27422745805597
H	8.50045875923748	19.87380720753645	9.03852166989607
H	7.08904640218786	20.25508766476164	9.56696429079414
O	11.61182013129009	15.03161903854519	9.24599704725899
H	10.90878185408303	14.35955542211630	9.09751680965381
H	12.44134328735436	14.51363080661617	9.21731394208421
O	11.31024782976947	9.55879374981968	9.19977038849980
H	10.77560701085415	8.76035250977406	8.88733445505878
H	12.13420591861785	9.19749886286479	9.56647606379441

12) Co-adsorbed H_1^+* and $H_2^+* + 2H_2O-OH^-* + 3H_2O^*$

Energy=-8801.17756065395

H	5.77741508853499	18.48719919980331	2.80454894173749
H	5.77741494449984	13.04046337397613	2.76833020447402
H	5.77741490975777	7.59242005932576	2.73413663464018
H	13.48063509253336	13.03905259675511	2.77042344505801
H	6.55859736763475	3.22350850899269	5.83627544132412
Ga	5.84025206413771	19.20997266320787	5.80940640942441
Ga	5.76393647102324	13.79649254209861	5.81501495803664
Ga	5.79551350029417	8.15038207158430	6.03442521099095
Ga	13.44017350193664	13.68064317181644	6.04232078950368
H	12.70392633629886	8.66726172495174	5.87242506730154
H	1.92580497303110	13.03905184442265	2.77042456552101
H	9.62902518720776	18.48719932699927	2.80454880500653
H	9.62902505200857	13.04046306677781	2.76833079128743
H	9.62902480053911	7.59242103141903	2.73413538970823
H	0.77682472895709	11.44172600332294	3.92960754675855
H	14.62961387653903	11.44172602765437	3.92960798913205
Ga	7.74189199871697	16.35977426404083	3.87774185840125
Ga	7.71375134666832	10.90474711444130	3.86655988155549

Ga	7.69365585266097	5.32639837334646	3.94283043829078
Ga	7.71138484249758	21.83538791030984	3.90486095107057
Ga	3.81509799412178	16.35207051798721	3.88780606435804
Ga	3.82384491089389	10.85467363179658	3.89861930583505
H	4.62962026501634	5.99564055596155	3.89357730483083
Ga	11.58113624979636	16.33789759932187	3.89717501985055
Ga	11.57802710062311	10.87610708484193	3.86929381977407
H	10.77682057862602	5.99563915977086	3.89357706072902
Ga	1.96308913502667	13.67303094485223	6.05366378346360
H	2.70251349970181	8.66726136938510	5.87242540627461
H	8.84784134936304	3.22350893660149	5.83627572742278
Ga	9.61036140138082	19.06919644310832	6.03055328341330
Ga	9.61766870423759	13.62965067593220	6.00405508553732
Ga	9.62326103701947	8.16150067867795	6.00794480056564
H	0.74840065595499	11.67346249571636	7.64098897699316
H	14.65803972401853	11.67346263186828	7.64098961387613
Ga	7.73687612625727	16.47444286394927	7.74455211718155
Ga	7.71101233773028	11.02377996525855	7.70644984150095
Ga	7.72729829078045	5.14648745893336	8.51173332535018
Ga	7.71111520286469	22.05330781908042	7.64322411789587
Ga	3.83753188599476	16.48251879429985	7.81099818762306
Ga	3.69346301656730	10.97947442976063	7.83324855456205
H	4.60139088683849	6.22734721931052	7.60533349302958
Ga	11.53014855394298	16.57828819081850	7.69553460524024
Ga	11.58983286305092	11.05194851233113	7.71947571202444
H	10.80504962454126	6.22734641056144	7.60533301704434
P	5.79130267385238	17.69880956982574	3.97433341945111
P	5.76035914740825	12.28395218876571	3.96174443116601
P	5.78597302343585	6.83634529030653	3.95266509028582
H	6.38704550516622	22.71684348300555	4.00420321456062
H	12.85194059900118	17.25642353404117	3.96807753434606
P	13.48169921213896	12.29130417261577	3.98801898964127
P	5.81057542437883	17.80281377398907	7.70895250877474
P	5.71073877327572	12.29935805996482	7.62541127989466
P	5.83356672933963	6.86428362476781	7.94872476647688
H	6.39778625755942	22.90385786230420	7.89512872377650
H	12.85064303955354	17.45114201383787	7.85597217673357
P	13.51138212378238	12.40891856176304	8.06860091877489
H	7.70321981496353	4.53002831093745	2.61196077858188
H	7.70322007447423	20.84237176109345	2.68056192850776
H	7.70322005289767	15.40326648805470	2.65531097839203
H	7.70321993525954	9.95986303264452	2.62421703938023
H	3.85161006084987	15.39798400310769	2.64793622181723
H	3.85160996956858	9.96381135041050	2.62972792579362
H	11.55483006647964	15.39798442629453	2.64793744487981
H	11.55482989397709	9.96381195691547	2.62972871406157
H	2.55450149756888	17.25642177770935	3.96807763020855
P	1.92638086677569	12.28921070293889	3.99088339614618
P	9.64180227646812	17.72430320343485	4.00580056584168

P	9.64825168423727	12.28836689737340	3.98021304307401
P	9.61391958887193	6.82639562767146	3.94895056761178
H	9.01939441622376	22.71684271581176	4.00420261652485
H	0.63926644212736	14.47657187807255	5.89317725452849
H	14.76717408724365	14.47657319097411	5.89317634541130
P	7.70706810964966	4.09861131886433	6.00404387544869
P	7.75246541856810	20.50817088108827	5.89083010336052
P	7.73152525440819	15.04986373786223	5.87613005130474
P	7.70530264783508	9.57433645124746	5.83870167941537
H	4.48384904900080	19.92840924157360	5.92900073132509
P	3.84446747691416	15.08714364182755	5.89365019518281
P	3.82096963351791	9.54628754000963	5.91542775737113
H	10.92259262272615	19.92841058996272	5.92900142982773
P	11.51118089309530	15.02945616405685	5.90438464759452
P	11.58436654284205	9.55404466652805	5.85479468203882
H	2.55579664855308	17.45114110378059	7.85597167416005
P	1.85784804981452	12.44801388294373	8.09138071291788
P	9.58965696480978	17.82810193843076	8.14706524504014
P	9.63129800888611	12.36906840083426	8.05904552873287
P	9.66707967367823	6.99361364704655	8.01154076093870
H	9.00865265306088	22.90385814274805	7.89512903073248
O	4.35424128185903	10.01865623368841	9.38159075881015
O	6.92930194480074	9.78453429347960	9.21785995204676
H	5.66958631721081	13.13007622840685	8.75995122911420
H	4.14404558599426	10.52469595212429	10.18269492901575
H	5.89955041815462	9.91708218635307	9.31132032148313
H	6.98581400783670	8.82387578014948	9.03212881688010
H	5.86779575631429	18.63725176188834	8.84579672159356
O	4.43669953935162	15.27930850686131	9.23326086607011
O	6.96813581646308	15.30424279231592	9.30102557243103
H	4.07566965650460	15.50470932806930	10.10381466434104
H	5.90288979956684	15.27128027359651	9.30147966008005
H	7.31410192651848	14.40379256442317	9.40496289182518
O	7.92325723208821	20.65030216058768	9.28150219170195
H	8.49633770702894	19.88191801461751	9.05404449776780
H	7.08371611529106	20.26575289254924	9.58012907905315
O	11.64961711278248	15.07471964661802	9.27611631276166
H	10.94111286838666	14.40320717855246	9.18332726992651
H	12.47698461439299	14.55385973180059	9.24434505747607
O	11.28858929374092	9.57965460913546	9.21840037800145
H	10.77703464351272	8.76679552694655	8.90281324128710
H	12.09732881461242	9.24096225771632	9.63743675778171

Species co-adsorption effect on adsorbed proton acidity

1) H₂O adsorption effect

Co-adsorbed H₁⁺* and H₂O

Energy=-8342.81786889163

H	5.77741506293526	18.48719917798028	2.80454898826884
H	5.77741495768782	13.04046327453027	2.76833029387022

H	5.77741496005906	7.59242013259344	2.73413663349260
H	13.48063515847460	13.03905254217737	2.77042347992248
H	6.55859727364865	3.22350849134130	5.83627542708858
Ga	5.80692202554292	19.13432321129276	5.98185622182209
Ga	5.78944272778644	13.72646473819154	5.87677461180408
Ga	5.77328184009747	8.22145388667989	5.94930992032271
Ga	13.46387532944526	13.69445248673928	6.04194633705185
H	12.70392633097620	8.66726172612499	5.87242512067101
H	1.92580492707135	13.03905179564362	2.77042455872965
H	9.62902520685438	18.48719934137429	2.80454881422410
H	9.62902509426382	13.04046301687190	2.76833070863350
H	9.62902479938489	7.59242111171275	2.73413533397824
H	0.77682475144987	11.44172602436703	3.92960753559799
H	14.62961383460524	11.44172607187953	3.92960796609281
Ga	7.71411792901008	16.36520266772197	3.86364034875635
Ga	7.73075447292200	10.94028051498145	3.81737711053567
Ga	7.70487534236760	5.40587423684495	3.85038665266382
Ga	7.70327077737802	21.84813587563750	3.88165537453031
Ga	3.82921449110800	16.36974779112065	3.86090381802439
Ga	3.81061338876424	10.89900890109515	3.83592793076970
H	4.62962022206323	5.99564051293318	3.89357731968496
Ga	11.58036396691732	16.35705208310098	3.87145317986195
Ga	11.59276538766123	10.89421471680836	3.84608197173749
H	10.77682060782938	5.99563913766669	3.89357709747309
Ga	1.94050907163492	13.69140284742764	6.02279704501291
H	2.70251343762618	8.66726133917965	5.87242544715601
H	8.84784144056371	3.22350889564485	5.83627573859082
Ga	9.60262588213275	19.13094422459260	5.98687309383951
Ga	9.63343678718329	13.65296573052220	6.01275535024093
Ga	9.65870418241282	8.22291721701521	5.94355404442266
H	0.74840064348578	11.67346250536902	7.64098896680875
H	14.65803976763508	11.67346261864790	7.64098959897494
Ga	7.70840857210329	16.68699055787065	7.54528053241787
Ga	7.86283083191771	10.97734336468227	7.66758652754495
Ga	7.71219182011407	5.76157736483077	7.55647616382750
Ga	7.70320187800280	22.19517632896228	7.44663419324328
Ga	3.91770381629311	16.75244803976404	7.50349538306831
Ga	3.60984141521756	11.14629564623691	7.58056799449386
H	4.60139089472083	6.22734725895234	7.60533348014436
Ga	11.49549780487631	16.73522372419325	7.50039550734684
Ga	11.68181427835550	11.21599828971307	7.58651815202879
H	10.80504969229926	6.22734636662090	7.60533302028335
P	5.78925165437024	17.72231383126967	4.00627587550945
P	5.76411498777682	12.28046127012071	3.96461395931807
P	5.77267565289255	6.84168468970369	3.94652045352176
H	6.38704559223251	22.71684348727315	4.00420320600051
H	12.85194063971174	17.25642361984326	3.96807756932369
P	13.49063793796814	12.29869649576471	3.99180148469449
P	5.81864508129485	17.89256541170412	8.11228207355970

P	5.76536556371241	12.15136178364887	7.75080042050606
P	5.74025631081381	7.00353794094561	7.98032612042087
H	6.39778589361151	22.90385776962766	7.89512877817089
H	12.85064302472369	17.45114201303614	7.85597215246779
P	13.57268148000213	12.46578426071906	8.10442957588711
H	7.70321979566987	4.53002828154633	2.61196082430271
H	7.70321993138839	20.84237166794549	2.68056180696545
H	7.70322006509616	15.40326646419317	2.65531095876101
H	7.70321994574026	9.95986308575149	2.62421698491432
H	3.85161014727175	15.39798381603701	2.64793601287195
H	3.85160997758630	9.96381138292347	2.62972781967473
H	11.55483003095905	15.39798435262348	2.64793740153031
H	11.55482986265075	9.96381204941591	2.62972873406020
H	2.55450137410119	17.25642190889366	3.96807773377788
P	1.91550370727596	12.29669762765915	3.98837516551659
P	9.62738179533367	17.72571945901023	4.00684522728644
P	9.65899890804534	12.30387864029755	3.98703434477048
P	9.63491813798088	6.84071726856530	3.94607926320804
H	9.01939450093776	22.71684277481646	4.00420264490915
H	0.63926658049166	14.47657186651812	5.89317729422417
H	14.76717398785915	14.47657314271559	5.89317633915168
P	7.70345637898098	4.06396450446358	5.86665445110450
P	7.70497054510217	20.48497890189461	5.90253331485089
P	7.72323823730581	15.02215953356157	5.89940419152038
P	7.71354418501122	9.57507208199040	5.78532583774912
H	4.48384906364475	19.92840924061548	5.92900074265145
P	3.87066677140230	15.03223495387860	5.90672350498487
P	3.80421182648297	9.55349899602941	5.86179934944357
H	10.92259276205989	19.92841066856393	5.92900142961504
P	11.52553879836986	15.02300930909314	5.90405124348308
P	11.60691400566082	9.56620200677888	5.87825760664812
H	2.55579641515330	17.45114121514204	7.85597177672678
P	1.81398859138611	12.48644367836446	8.11539187248537
P	9.59647270920243	17.89081709513870	8.10945970558422
P	9.68542258018613	12.36902708033418	8.06963852155780
P	9.67315271928042	7.01232247907764	7.98516079439745
H	9.00865301037593	22.90385829480549	7.89512909178832
O	7.62884614177064	9.57775670684005	9.22153157834116
H	8.39664951818908	9.00716641440184	9.41554522765363
H	6.84240904930518	8.99561098133348	9.23312851502032
H	5.73005683499375	12.99502768301482	8.87512518363619

Adsorbed H₂O

Energy=-8342.36869916855

H	5.77741505517545	18.48719916595434	2.80454898125835
H	5.77741494902231	13.04046329421139	2.76833022902675
H	5.77741497078737	7.59242013837246	2.73413663530586
H	13.48063510011931	13.03905257669249	2.77042346476494
H	6.55859727258876	3.22350850189642	5.83627542513067

Ga	5.80373528637538	19.12473533727102	5.98519789614344
Ga	5.78460876206590	13.65811738260988	6.01413731715188
Ga	5.76575785396325	8.24250384282266	5.94724552712301
Ga	13.46026368505507	13.69503732731921	6.03904334543566
H	12.70392631859337	8.66726172377668	5.87242510440112
H	1.92580496848618	13.03905182636089	2.77042456424781
H	9.62902520576375	18.48719934098871	2.80454881379305
H	9.62902506013454	13.04046304607271	2.76833077250128
H	9.62902480983430	7.59242109919586	2.73413533657227
H	0.77682474024129	11.44172601334248	3.92960756959587
H	14.62961386871156	11.44172604612106	3.92960798541946
Ga	7.70324056945101	16.34942023303439	3.87756642798050
Ga	7.70321048875378	10.93893853931223	3.82504923311436
Ga	7.70303079535400	5.41367444811986	3.84690595237890
Ga	7.70318919061093	21.84411053179631	3.88658488203704
Ga	3.82916573701487	16.35660855881883	3.87466489523254
Ga	3.83006067525060	10.89674757901811	3.84801053438365
H	4.62962021119134	5.99564050469402	3.89357732254539
Ga	11.57725739062812	16.35648221313140	3.87478611850778
Ga	11.57625761731919	10.89656437150201	3.84813699677672
H	10.77682058855967	5.99563915337011	3.89357709415850
Ga	1.94650561023370	13.69551898558467	6.03904920680632
H	2.70251342876756	8.66726133088834	5.87242544086203
H	8.84784144416330	3.22350889436278	5.83627573930852
Ga	9.60274201029293	19.12463145085905	5.98516863733150
Ga	9.62165137377614	13.65804513113343	6.01423269029478
Ga	9.64055873877583	8.24266459987014	5.94764889057033
H	0.74840068017458	11.67346251714084	7.64098898204003
H	14.65803973158865	11.67346262912696	7.64098961660394
Ga	7.70325198176314	16.67065033393195	7.53736891707996
Ga	7.70293063694946	11.06910172302558	7.63770062352558
Ga	7.70327439058030	5.76749384618553	7.55107905056128
Ga	7.70323752212045	22.19083460955860	7.44650364333349
Ga	3.91225244842776	16.73302463697313	7.49604754278825
Ga	3.75646000821560	11.22400488543507	7.57291866208929
H	4.60139089417698	6.22734725372043	7.60533347860055
Ga	11.49446304954148	16.73267194857695	7.49554524732473
Ga	11.64998686946053	11.22408873525478	7.57317253399827
H	10.80504969458717	6.22734636980285	7.60533301842336
P	5.78589954985669	17.72053066121809	4.00490253900507
P	5.76020547487567	12.30301871100838	3.98659462366565
P	5.77079395499378	6.84455348852516	3.94956109989322
H	6.38704556692015	22.71684351565242	4.00420322206001
H	12.85194065309711	17.25642361573164	3.96807758275849
P	13.48620037427225	12.29515451270988	3.99030087875521
P	5.81422069395351	17.88476156550098	8.10720717449448
P	5.75790728517689	12.35007148823167	8.03733629579670
P	5.73702529855264	7.00833798669602	7.97937765696108
H	6.39778566172486	22.90385776499240	7.89512883401651

H	12.85064303203714	17.45114199413831	7.85597214812475
P	13.56034878784305	12.45812878838542	8.09531759938347
H	7.70321979754871	4.53002827921359	2.61196081537731
H	7.70321986959354	20.84237155824610	2.68056168430100
H	7.70322006519764	15.40326644700830	2.65531094365241
H	7.70321994967789	9.95986305716095	2.62421699314885
H	3.85161013636501	15.39798385914962	2.64793606072310
H	3.85160997130407	9.96381136283609	2.62972780948193
H	11.55483002163245	15.39798434906018	2.64793739675912
H	11.55482987590247	9.96381197069482	2.62972869655550
H	2.55450141330630	17.25642187188099	3.96807772352888
P	1.92014466874789	12.29530992312943	3.99034172292596
P	9.62055170693015	17.72050954405613	4.00488867364252
P	9.64620135278462	12.30297722545893	3.98659408368822
P	9.63561400965809	6.84447733273810	3.94949016962325
H	9.01939460834981	22.71684284421222	4.00420267591430
H	0.63926648605279	14.47657187020412	5.89317725193803
H	14.76717412002607	14.47657320788648	5.89317634477174
P	7.70320698699060	4.06513266054951	5.86334101254648
P	7.70328067174262	20.48074371964691	5.90347689935484
P	7.70318542754164	15.01110654193735	5.89599596385307
P	7.70314538130291	9.58487324591803	5.79279647897898
H	4.48384905483295	19.92840924106991	5.92900074439698
P	3.88343977036970	15.02310236185603	5.89971828640463
P	3.80264805386290	9.56272756216131	5.87554244666422
H	10.92259272627338	19.92841064525822	5.92900143379976
P	11.52315848811002	15.02264043466417	5.89966905180072
P	11.60380560174930	9.56271794445949	5.87557978301756
H	2.55579640979245	17.45114121718837	7.85597177814396
P	1.84614097928649	12.45802654812924	8.09517408981662
P	9.59248826427413	17.88442008542100	8.10701403144837
P	9.64826080829117	12.34960867129644	8.03729926914523
P	9.66947487284694	7.00828547730693	7.97967226528523
H	9.00865323143087	22.90385835680560	7.89512912285375
O	7.70230514401511	9.59353561337146	9.19868838812446
H	8.48407489635825	9.01247021778656	9.26620627790420
H	6.92318679101077	9.00859400402348	9.26306361248690

2) o-DHP adsorption effect

Co-adsorbed H_1^+ * and o-DHP

Energy=-8515.7485360242

H	-1.91661999896570	5.25587699679341	-3.17390100461669
H	-1.91344800501672	-0.19092898523298	-3.19943400122568
H	-1.91027411465485	-5.63904013214320	-3.22293894150362
H	5.78977399893501	-0.18780599394231	-3.20391000587482
H	-1.12387494794212	-10.00140603285277	-0.11289602158648
Ga	-1.88516905392848	5.90811864059582	0.00178567288135
Ga	-1.89938308032781	0.53353331335837	-0.12452111527825
Ga	-1.90352402061098	-5.00471608624058	0.00368290449327

Ga	5.77278334042378	0.47852618814402	0.06014812801872
H	5.01828398789968	-4.55396801264734	-0.09266999368753
H	-5.76505605016630	-0.19460102985848	-3.19404999808255
H	1.93498999990908	5.25814199481253	-3.17718800416782
H	1.93816199904965	-0.18866498636000	-3.20271999786937
H	1.94133599498787	-5.63677402675445	-3.22622697589000
H	-6.91210694850772	-1.79032896139980	-2.03075301149871
H	6.94068200468174	-1.78218200515498	-2.04257299991845
Ga	0.02600104345042	3.14362554469851	-2.11781683983154
Ga	0.04007145521414	-2.30045571846689	-2.12698180133789
Ga	0.02018054485176	-7.81691129512384	-2.10698162905861
Ga	0.00818767288719	8.61947032829095	-2.10440449118762
Ga	-3.86429759903688	3.14264089817926	-2.11544504285903
Ga	-3.87332660072308	-2.33320122150197	-2.12288410639791
H	-3.05613984996758	-7.23421886447173	-2.05938603994658
Ga	3.88873938662893	3.13343541421044	-2.10994406548291
Ga	3.90292972485063	-2.33306531364319	-2.12089162845076
H	3.09105998733417	-7.23060498547324	-2.06463199989496
Ga	-5.74925055613730	0.46183128860924	0.05383710014583
H	-4.98313002293146	-4.55985001772384	-0.08413500101663
H	1.16536992116180	-10.00005895691557	-0.11484898986564
Ga	1.91094260584057	5.90800660753828	0.00477438028483
Ga	1.94580770782182	0.43317607515255	0.02298388456545
Ga	1.96558133763857	-4.99220103918848	-0.00189592454499
H	-6.94352701222098	-1.57782001815790	1.68020000069134
H	6.96601000304321	-1.54180799993981	1.63848100004840
Ga	0.01951908728844	3.46544318210464	1.56695644372190
Ga	0.14693962805744	-2.21425509801308	1.78359860904463
Ga	0.03614833984096	-7.47184720317304	1.59106246213179
Ga	0.01091539593403	8.97379071387410	1.45943439139281
Ga	-3.77262694888856	3.52846254756905	1.52686443615133
Ga	-4.06089813540257	-2.05422516859292	1.59731342414371
H	-3.08133794995266	-6.99524697576213	1.65193898137474
Ga	3.80716378162872	3.51699633358711	1.51704467507452
Ga	3.98926972178189	-1.98617600288286	1.60107092825579
H	3.12232098996107	-6.99160000667127	1.64664600204503
P	-1.90317284664657	4.49350130001899	-1.97169961667860
P	-1.92346095456380	-0.94611406229895	-2.00306968661255
P	-1.91407150957315	-6.38402794893269	-2.00691246904313
H	-1.30845398174181	9.48823399652184	-1.98306500463040
H	5.15962199070200	4.03154499446820	-2.01399400742872
P	5.80087489375490	-0.92621553178582	-1.98148594570021
P	-1.87131008708868	4.66949406893519	2.13435428612100
P	-1.93129873755766	-1.00526599466189	1.73570319154450
P	-1.93339035811718	-6.23840062715846	2.02013481303670
H	-1.29450304662306	9.68288800103073	1.90748500788226
H	5.16152700238484	4.23389000042110	1.87351900338485
P	5.88817838790433	-0.75172470831099	2.12193518782568
H	0.01722798824460	-8.70053798583874	-3.34075001618131

H	0.00769299452714	7.61193900489047	-3.30415200231820
H	0.01086999899201	2.17278500087531	-3.31873100319359
H	0.01404499766293	-3.27067901424843	-3.33914599310374
H	-3.84074299982809	2.16522299912983	-3.32281000559975
H	-3.83756199817169	-3.26898599925630	-3.33035699660715
H	3.86247800530369	2.16975300912307	-3.32938199635317
H	3.86565800603778	-3.26445500497825	-3.33692899975455
H	-5.13781700283266	4.02548800285393	-2.00520699871358
P	-5.77259856999499	-0.93666252464501	-1.97576103789181
P	1.93693016260010	4.50162646531890	-1.97404693407331
P	1.96760454220352	-0.92638517943853	-1.98570453427634
P	1.94972153319213	-6.38071993052488	-2.00840214455614
H	1.32389498647723	9.48978098913558	-1.98531200232108
H	-7.04977497653042	1.24828800986021	-0.07301999963013
H	7.07813298473146	1.25659799163262	-0.08507599875444
P	0.02160605397610	-9.16313019594074	-0.09237226715865
P	0.01209073929177	7.26018341655741	-0.08103417568651
P	0.04079153501036	1.81128790314370	-0.08636330326566
P	0.02355424680315	-3.62882860299776	-0.12050231345950
H	-3.20836799989937	6.70245699770788	-0.05117200342373
P	-3.82833621392904	1.81541563556968	-0.07326529484503
P	-3.87769724061315	-3.67622492102455	-0.09292799394211
H	3.23037599158144	6.70624499665709	-0.05666599964590
P	3.83641624750068	1.80671711870252	-0.07930748664572
P	3.91939776111996	-3.65641325076757	-0.08656721656517
H	-5.13331999846245	4.22783499861503	1.88230399806820
P	-5.88186058391948	-0.75193605733264	2.14796288318256
P	1.90817131978977	4.67092446398149	2.13099752783400
P	2.00332140663026	-0.82397870183601	2.07935262464396
P	1.98934520223881	-6.21094044018249	2.03577784033532
H	1.31636404363954	9.68442401160148	1.90525700396026
C	-1.81036794920532	-2.30224285436506	4.88112286628645
C	-1.54029713929602	-3.32621552371449	4.05694298292057
C	0.83419240255127	-3.14193055960077	4.57243102614118
C	0.54013468142593	-1.76600071017347	5.11534603507197
C	-0.74138170327274	-1.38528009658268	5.27224392008718
H	-0.99984240930034	-0.42492882949908	5.70542412726332
H	1.37227174469955	-1.14300421437649	5.42023453841464
H	0.78555687876600	-3.89577200008983	5.37000908712147
H	-2.26156447745039	-4.04179189300461	3.68641178213149
H	-2.82297211665613	-2.14585656102427	5.23503373969890
N	-0.19277715120140	-3.47800596364527	3.53452577812940
H	-0.06131601713760	-4.45139418939294	3.25367209072648
H	1.81768767059356	-3.19808650191018	4.10272112527219
H	-1.99982131340126	-0.17928331783296	2.87128196367249

Adsorbed o-DHP

Energy=-8515.29655222234

H	5.77741510482199	18.48719913429732	2.80454891492926
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H	5.77741498963069	13.04046330934358	2.76833018649507
H	5.77741487876274	7.59242005213041	2.73413667600804
H	13.48063513974616	13.03905257217330	2.77042345282988
H	6.55859720229205	3.22350856738579	5.83627543634115
Ga	5.80329393493846	19.12348834061107	5.98482225950254
Ga	5.78363882594719	13.66965938671592	5.98675830945942
Ga	5.77370264307130	8.24872255660391	5.96077281698130
Ga	13.45692666344762	13.70139918029987	6.03349048927113
H	12.70392635996757	8.66726176414295	5.87242506332829
H	1.92580490553160	13.03905176595875	2.77042463091440
H	9.62902515376703	18.48719928814478	2.80454879574622
H	9.62902502277429	13.04046300689125	2.76833076925418
H	9.62902495747420	7.59242095062585	2.73413538849448
H	0.77682480772918	11.44172608375783	3.92960751881169
H	14.62961384130395	11.44172605435371	3.92960799106069
Ga	7.70425977506234	16.35474603980913	3.87287127133234
Ga	7.70240555428167	10.92459102986191	3.84747751734382
Ga	7.70400887723122	5.41988442659701	3.84362557016576
Ga	7.70312977012195	21.84405341378859	3.88666035563646
Ga	3.82697485443604	16.35844969569562	3.87210019676618
Ga	3.83196768617943	10.89334437056922	3.85264552427242
H	4.62962030358752	5.99564059195171	3.89357730511412
Ga	11.57738306674644	16.36025834762122	3.87100983579175
Ga	11.57593556646557	10.89525878346062	3.84949493323423
H	10.77682042157203	5.99563929323788	3.89357704680571
Ga	1.94468935952409	13.69271342035601	6.03847041460712
H	2.70251338367701	8.66726127165434	5.87242542855138
H	8.84784154780801	3.22350882754815	5.83627573936809
Ga	9.60234079146910	19.12496763055624	5.98516926665955
Ga	9.62360734139164	13.66545603769530	5.99074010816763
Ga	9.63002656191530	8.25274638690430	5.96890354888727
H	0.74235903978640	11.64697401004234	7.64093316715797
H	14.65193822945341	11.67486488273705	7.61113872201739
Ga	7.70356493426338	16.66783538915783	7.53080823364334
Ga	7.68600427890599	11.11572656173512	7.73039895026194
Ga	7.70986043422812	5.75765154705216	7.54077693430928
Ga	7.70320363241189	22.19027813345270	7.44701611399442
Ga	3.91006769631474	16.73079306715325	7.48991047225469
Ga	3.77151293861745	11.24940473662355	7.57113433206118
H	4.60139081272906	6.22734722311389	7.60533346756464
Ga	11.49467332205655	16.73405689577115	7.49133408624477
Ga	11.64138325058502	11.24568639843092	7.55558119843188
H	10.80504967580744	6.22734640728929	7.60533304385766
P	5.78500189376280	17.72081483726268	4.00378887058547
P	5.76163685350469	12.30025787524719	3.98232163777955
P	5.77006059204798	6.84960051249092	3.95281364159593
H	6.38704568607183	22.71684347101522	4.00420320251013
H	12.85194059996167	17.25642353063251	3.96807755460211
P	13.48615087863218	12.29501876396886	3.99006291115411

P	5.81353245924162	17.87953024633940	8.10551303813417
P	5.74277565203674	12.42506723417663	8.01740795941802
P	5.74445317183041	6.99130631312762	7.97605821806230
H	6.39778574714411	22.90385777455532	7.89512880231842
H	12.85064303326284	17.45114199207455	7.85597217933946
P	13.56188079757459	12.45764733228849	8.08631387626916
H	7.70321980821153	4.53002828698417	2.61196077085676
H	7.70321989709469	20.84237166630933	2.68056180262654
H	7.70322005983099	15.40326654590253	2.65531098742131
H	7.70321994220675	9.95986320291710	2.62421712198191
H	3.85161004820394	15.39798400175415	2.64793616130655
H	3.85160995019421	9.96381137226852	2.62972784678484
H	11.55483006343723	15.39798442568061	2.64793742382766
H	11.55482988268158	9.96381194830063	2.62972866426765
H	2.55450152508554	17.25642176979785	3.96807765946527
P	1.92087903874994	12.29370951622785	3.98977938408212
P	9.62112886871972	17.72244984456839	4.00394749040659
P	9.64472932402091	12.29902575446378	3.98253244333746
P	9.63675431243064	6.85113827504188	3.95509838150205
H	9.01939446081483	22.71684277062405	4.00420264534404
H	0.63926650899765	14.47657184568818	5.89317724143022
H	14.76717406901419	14.47657318340526	5.89317634043141
P	7.70406348634511	4.06250517649968	5.85642886375241
P	7.70262817637790	20.48046611160122	5.90387508501264
P	7.70489458537565	15.01863182323390	5.88233110685022
P	7.69944522820413	9.61610322512998	5.85783494499946
H	4.48384897391726	19.92840928318719	5.92900073558040
P	3.87697277603079	15.02735613413813	5.88943957569639
P	3.80509509701098	9.56442489635150	5.88610763634333
H	10.92259262787518	19.92841060081648	5.92900142540360
P	11.52426124408868	15.03096696180409	5.89021598858458
P	11.60153103401820	9.56239809543004	5.87827150985893
H	2.55579665202190	17.45114111733178	7.85597169240729
P	1.83412966021817	12.44478445643284	8.09265280310226
P	9.59142163683382	17.88215596188682	8.10714254527337
P	9.65824431955979	12.39469774084927	8.01819541723352
P	9.67015520678859	7.00315325763734	7.99348426700375
H	9.00865315191435	22.90385832259270	7.89512910391923
C	6.19212294023905	10.77382091383354	11.07230578000696
C	6.33796562694101	9.83712115388280	10.12380073153619
C	8.76821470198477	9.92874020308088	10.35879973123617
C	8.57487038224809	11.22860974590365	11.09871908170091
C	7.33302183319726	11.60620262116428	11.45118320211212
H	7.15731821646986	12.51221266136495	12.02233600004032
H	9.45428979998741	11.79744143519964	11.37763281511565
H	8.83123168996560	9.08514448501426	11.06136761217334
H	5.54789772887777	9.20176815035451	9.74643155257824
H	5.22403564905490	10.92824814375129	11.53457420297422
N	7.60876696203296	9.71039384926457	9.44068121640349

H	7.68248457091465	8.76873056433446	9.05576532731784
H	9.67682192288204	9.93250413463810	9.75444969739337

3) Py adsorption effect

Co-adsorbed H_1^+ and Py

Energy=-8514.5814913007

H	5.77741507556606	18.48719924691621	2.80454892767121
H	5.77741499117657	13.04046336176839	2.76833028873247
H	5.77741486039999	7.59242003644617	2.73413667546678
H	13.48063514905732	13.03905253238169	2.77042348294233
H	6.55859731075671	3.22350848996883	5.83627543335213
Ga	5.80653980934736	19.13431420939326	5.98224979058866
Ga	5.78839903148123	13.73269613834257	5.86540880534928
Ga	5.78404248745931	8.21915084221329	5.98582961972656
Ga	13.46379424661419	13.69648293565480	6.03583915890658
H	12.70392628313940	8.66726177285125	5.87242508341260
H	1.92580490595558	13.03905173500654	2.77042463031544
H	9.62902519049353	18.48719934264937	2.80454880977963
H	9.62902506144486	13.04046303940721	2.76833073981623
H	9.62902496088991	7.59242095353660	2.73413539765657
H	0.77682476850022	11.44172608699049	3.92960747655991
H	14.62961382095943	11.44172608327621	3.92960797055213
Ga	7.71302473701615	16.36801860316771	3.86136770774904
Ga	7.72999782238604	10.92164952699348	3.84466203430163
Ga	7.70375934480073	5.40910422011060	3.85198573485582
Ga	7.70324880192285	21.84825680395999	3.88161939544557
Ga	3.82865120252590	16.37091156632053	3.85952748120231
Ga	3.81351511256627	10.89646941833530	3.83885442024922
H	4.62962034734101	5.99564061271309	3.89357730696545
Ga	11.58133343463576	16.36129270964258	3.86691560149818
Ga	11.59038069557072	10.89100160542972	3.84940210727475
H	10.77682042606625	5.99563929320751	3.89357707057944
Ga	1.94146260911874	13.69463680066595	6.01980030623506
H	2.70251344253763	8.66726133979050	5.87242544222836
H	8.84784141093957	3.22350891506252	5.83627574421390
Ga	9.60243489914093	19.13145482940504	5.98602643668907
Ga	9.63948620072056	13.66557152352154	5.98913411294820
Ga	9.64912703342251	8.22336969105827	5.97265697269623
H	0.74840064867620	11.67346250428285	7.64098895968440
H	14.65803973080867	11.67346262434614	7.64098961206308
Ga	7.70757806541993	16.68709786765189	7.54206957936638
Ga	7.87221119398817	11.00756503526259	7.75996374382736
Ga	7.70928165093242	5.76869097098181	7.56393075331419
Ga	7.70321826132574	22.19521054743837	7.44692124698188
Ga	3.91731252761754	16.75167326113468	7.50273111586995
Ga	3.60995015130542	11.16247287584547	7.56423098938984
H	4.60139087506004	6.22734725512526	7.60533347769737
Ga	11.49603995003248	16.73813872423271	7.49528006852932
Ga	11.68141809862807	11.23782743829346	7.57018634971488

H	10.80504970761029	6.22734636450662	7.60533301791169
P	5.78849089085124	17.72325679235310	4.00588412946000
P	5.76649298375776	12.27799883902316	3.96375187423119
P	5.77144758964451	6.84884313972662	3.95389516434428
H	6.38704562989944	22.71684348030494	4.00420320999592
H	12.85194066508586	17.25642360541024	3.96807756655088
P	13.48937705197210	12.29704410440001	3.99082825555670
P	5.81850839891667	17.89199071675850	8.11256803850858
P	5.75849934639789	12.17915514717360	7.74919064812262
P	5.73001184624752	6.99599765774799	8.01076170309686
H	6.39778592867527	22.90385780116128	7.89512876268341
H	12.85064294769462	17.45114206375338	7.85597213149988
P	13.57568146935478	12.47043300477604	8.10270172673477
H	7.70321977716266	4.53002826110585	2.61196073691906
H	7.70321994963750	20.84237170558257	2.68056186230498
H	7.70322005119439	15.40326649498003	2.65531098726187
H	7.70321991948500	9.95986312597581	2.62421710059040
H	3.85161007215414	15.39798396563430	2.64793621943514
H	3.85160996656990	9.96381133779299	2.62972785069802
H	11.55483002595404	15.39798436031496	2.64793740241834
H	11.55482988776368	9.96381198575356	2.62972869455337
H	2.55450145491959	17.25642181643693	3.96807761974532
P	1.91665113005781	12.29550615437370	3.98807177457681
P	9.62719354765248	17.72639172585448	4.00612048628608
P	9.65656329960747	12.30019573681830	3.98425611720626
P	9.63550271253769	6.84695797729062	3.95223571337626
H	9.01939444289307	22.71684275269398	4.00420263442389
H	0.63926648322260	14.47657187443199	5.89317727904960
H	14.76717406806189	14.47657316913242	5.89317633853718
P	7.70354508777374	4.06548675912824	5.87049012078400
P	7.70467719064536	20.48523562110914	5.90275647601256
P	7.72323818702673	15.02694665411880	5.89308085713566
P	7.71332979613505	9.59824115372354	5.85348859672296
H	4.48384924704583	19.92840920093936	5.92900069449280
P	3.86951671831750	15.03650689776105	5.90176192697451
P	3.80872503666415	9.54998783192842	5.86588977774206
H	10.92259239928404	19.92841045978198	5.92900144982612
P	11.53142355383804	15.03256582913056	5.89369854521136
P	11.60363277530101	9.56448578562370	5.88345742895713
H	2.55579676786714	17.45114105863304	7.85597164128082
P	1.81251352481359	12.48982345815786	8.11393555748298
P	9.59623918339886	17.88976027552280	8.10924942449485
P	9.70492435166761	12.42025421155087	8.04434520911567
P	9.68047502475516	7.00547194636510	8.00757662761274
H	9.00865297061610	22.90385827563611	7.89512908053914
C	8.87296877244943	8.83266833477217	11.35567594739297
C	8.88336507095029	9.55162780780698	10.16988717150672
C	6.55685456238658	9.52815925268504	10.05988775438042
C	6.46830237290989	8.81136383178224	11.24457279566274

C	7.64550477595583	8.45497737795863	11.90339977309522
H	7.60646873686103	7.89249688632220	12.82926730669470
H	5.49615085146250	8.53341055627981	11.63202171247877
H	5.67172056750271	9.82853955386837	9.51522771143982
H	9.80926736751082	9.87900597565298	9.71416192962015
H	9.80930534000851	8.57143745826109	11.83249521421338
N	7.74296615189319	9.89572810148090	9.53043452954129
H	5.67658657861774	13.03898847560467	8.85980460485305

Adsorbed Py

Energy=-8514.13037996144

H	5.77741506112705	18.48719926415076	2.80454894676544
H	5.77741497979592	13.04046335424544	2.76833020960259
H	5.77741487747546	7.59242006379105	2.73413666318805
H	13.48063519302826	13.03905251271474	2.77042348961647
H	6.55859722649882	3.22350852957073	5.83627543570890
Ga	5.80396112021064	19.12576846775560	5.98536245954091
Ga	5.78096083712400	13.66869596237363	5.99364544108850
Ga	5.77563493434853	8.24239708636595	5.98349136379988
Ga	13.45982315130496	13.69867038572776	6.03678684647936
H	12.70392628993292	8.66726178048873	5.87242509883516
H	1.92580485069785	13.03905168734938	2.77042472842549
H	9.62902520165549	18.48719936152931	2.80454882434647
H	9.62902505264252	13.04046304119841	2.76833076816159
H	9.62902492380467	7.59242099270903	2.73413536564964
H	0.77682484500350	11.44172616367669	3.92960744892422
H	14.62961378688468	11.44172611283263	3.92960796779552
Ga	7.70330256571655	16.35374241292216	3.87438680547656
Ga	7.70313404599632	10.91987217821083	3.85319934143095
Ga	7.70287698299559	5.41748289598185	3.84833333708134
Ga	7.70313154109393	21.84467312072441	3.88617957385748
Ga	3.82837733900231	16.36045140293483	3.87102838213919
Ga	3.83115286265072	10.89450619576042	3.85096259480823
H	4.62962030953008	5.99564058882945	3.89357731213044
Ga	11.57811317473285	16.36022084778382	3.87125570549388
Ga	11.57470228684213	10.89411820771794	3.85137823368547
H	10.77682046445240	5.99563926058343	3.89357708448529
Ga	1.94741670221271	13.69986939578294	6.03730935422431
H	2.70251341659424	8.66726131670589	5.87242543308580
H	8.84784150290781	3.22350887435928	5.83627574476510
Ga	9.60251184158918	19.12569352257951	5.98531178169887
Ga	9.62534595951173	13.66888211533725	5.99395382247408
Ga	9.63059648908467	8.24257292711582	5.98334219177306
H	0.74840062188972	11.67346248673518	7.64098896771515
H	14.65803976615527	11.67346260623883	7.64098960926883
Ga	7.70320793126738	16.66981704016748	7.53336949438173
Ga	7.70291098887386	11.10608261258402	7.72839901383206
Ga	7.70311140800731	5.77642657224128	7.55916642837004
Ga	7.70322741289055	22.19162618950420	7.44605079885369

Ga	3.91148793447179	16.73542444937062	7.49156327761973
Ga	3.75861957718455	11.24356905670077	7.55836371286835
H	4.60139085157843	6.22734724971583	7.60533347720649
Ga	11.49545722848022	16.73486817126670	7.49086951876757
Ga	11.64782350074332	11.24362946785627	7.55901248383732
H	10.80504972212736	6.22734636082231	7.60533301758007
P	5.78551627659225	17.72214301670870	4.00448570868784
P	5.76219459238563	12.29952791313915	3.98422389710557
P	5.76927530954519	6.85165260481059	3.95705070072067
H	6.38704558193017	22.71684349060253	4.00420321728380
H	12.85194071389570	17.25642366084060	3.96807758276630
P	13.48603098155400	12.29447909284072	3.99022505010409
P	5.81442868793533	17.88435499205681	8.10686469876232
P	5.74188984380732	12.39929693616544	8.01946111616397
P	5.72674636672190	7.00163344175203	8.00814950408773
H	6.39778603967897	22.90385781890836	7.89512873562255
H	12.85064294809150	17.45114206142424	7.85597212998831
P	13.56283928304391	12.46100418384114	8.09447827040064
H	7.70321979445401	4.53002826700834	2.61196076065931
H	7.70322000599030	20.84237173497090	2.68056189762649
H	7.70322005102352	15.40326646139629	2.65531096549154
H	7.70321992639114	9.95986312376111	2.62421709699418
H	3.85161010315393	15.39798393977262	2.64793623945912
H	3.85160995008972	9.96381139265628	2.62972789308734
H	11.55482999806267	15.39798431533160	2.64793737580228
H	11.55482987909397	9.96381198983687	2.62972868854158
H	2.55450140437708	17.25642186065525	3.96807761541015
P	1.92014062429383	12.29484578625728	3.99050026536315
P	9.62103564899652	17.72212746773263	4.00449733724956
P	9.64403211034549	12.29961219908037	3.98433526458880
P	9.63708530851668	6.85144536753064	3.95685281764564
H	9.01939441836801	22.71684272743641	4.00420262522555
H	0.63926654564232	14.47657182592818	5.89317720185488
H	14.76717402514358	14.47657315046839	5.89317633829850
P	7.70318805127388	4.06642705333268	5.86764559908269
P	7.70327213549377	20.48211281318432	5.90306058286650
P	7.70315792545916	15.01742185817961	5.88720687399160
P	7.70302386783952	9.60902604244330	5.86047636406189
H	4.48384925889130	19.92840919599140	5.92900069230524
P	3.87953222866830	15.03185645849958	5.89033891293967
P	3.80609256065982	9.56031731969574	5.88045941968033
H	10.92259238927830	19.92841045989879	5.92900144266527
P	11.52751723306735	15.03102106572243	5.89048987813324
P	11.60024675345203	9.56022062958515	5.88056397261775
H	2.55579675701104	17.45114107519247	7.85597164919935
P	1.84384257224472	12.46091664277742	8.09429925236510
P	9.59240168106070	17.88362669022299	8.10661364544732
P	9.66418840074625	12.39852015078045	8.01980423106989
P	9.67956793604657	7.00159000777061	8.00784667286930

H	9.00865287234098	22.90385824123671	7.89512906357703
C	8.90596135812421	8.82820504341936	11.26212799409033
C	8.86482326805759	9.55901803380414	10.08246126817749
C	6.54070452856517	9.55975811541303	10.08312360021285
C	6.49979015273840	8.82882902996217	11.26275114924391
C	7.70294203307327	8.45584071430607	11.86364907463076
H	7.70305709451191	7.88385922501916	12.78479073160038
H	5.54452878469745	8.55381108341505	11.69268039822911
H	5.63495601306427	9.87988134361075	9.58378891418325
H	9.77045122723401	9.87909544797843	9.58291723557761
H	9.86132769184385	8.55352108268393	11.69205581657740
N	7.70270940675063	9.92239355760752	9.50209234853749

4) Py+H₂O adsorption effect

Co-adsorbed H₁⁺* and Py+H₂O

Energy=-8591.0129339921

H	-1.89126800096389	5.22936299041953	-3.08239700797970
H	-1.89129300830341	-0.21736691668970	-3.11949103203700
H	-1.89131801849913	-5.66540502151589	-3.15456000225407
H	5.81192803447671	-0.21877901285889	-3.12273899558611
H	-1.10798498206788	-10.03481499583191	-0.05366498237477
Ga	-1.86103497150731	5.87263375508625	0.09562703833149
Ga	-1.89232952262123	0.44065763904482	0.00927560747770
Ga	-1.90507723317835	-5.01447486816050	0.07564577012146
Ga	5.79621600834684	0.43957889749395	0.13795039617826
H	5.03736901968096	-4.59106699534932	-0.02090003926635
H	-5.74290200422081	-0.21877799517982	-3.11472601522615
H	1.96034200323424	5.22936296961042	-3.08506698752662
H	1.96031700821894	-0.21736796428699	-3.12216001679004
H	1.96029200092625	-5.66540401169422	-3.15723098151848
H	-6.89107801279856	-1.81629000543571	-1.95500301809114
H	6.96171098163080	-1.81629197766909	-1.96460701226369
Ga	0.03725219131459	3.10324530009597	-2.02100770537419
Ga	0.05617409182208	-2.33709796043925	-2.04142901166302
Ga	0.03694031033282	-7.84781654515973	-2.03855064900454
Ga	0.03523503315412	8.58921352067497	-2.00500656683460
Ga	-3.84129804484284	3.10321587872084	-2.01669157235479
Ga	-3.86106780947026	-2.36128720172185	-2.04490513332299
H	-3.03830900163176	-7.26237000034099	-1.99458000868438
Ga	3.91183400475520	3.10641996886066	-2.02685069653715
Ga	3.91782358799385	-2.36711110524555	-2.04197949720998
H	3.10889199898280	-7.26237199560390	-1.99884200189114
Ga	-5.72962557886273	0.41337698013653	0.16422364311888
H	-4.96404292155658	-4.59106695382053	-0.01396702166660
H	1.18125897844209	-10.03481398095333	-0.05525199644674
Ga	1.93543333424883	5.87146004323799	0.09371870095069
Ga	1.97148898233655	0.41931189118659	0.08588460450223
Ga	1.97906875310732	-5.02977434787731	0.07907517001241
H	-6.91692894730737	-1.58514998592463	1.75643500623390

H	6.99270994437815	-1.58515196498136	1.74679199302024
Ga	0.03936252673764	3.42178083835770	1.64899583583788
Ga	0.21717802550315	-2.22973484143492	1.87741753494672
Ga	0.04581142550057	-7.47981154005157	1.68068461438108
Ga	0.03776096344949	8.93555102629911	1.55863198888888
Ga	-3.75025306672230	3.48472976121098	1.61423831820683
Ga	-4.06085271960188	-2.24469884956194	1.85120648640909
H	-3.06396402460016	-7.03126002100581	1.71723300078274
Ga	3.83058761581116	3.47963818716641	1.60032687571270
Ga	4.01698060531755	-2.00680607469755	1.66920219051293
H	3.13969401922774	-7.03126101014738	1.71293200678402
P	-1.88327466006816	4.46382416316351	-1.88118506473110
P	-1.90588875565750	-0.98183717417776	-1.92262300172729
P	-1.89588715621438	-6.40964067782214	-1.93553470485144
H	-1.28080399617975	9.45881399572966	-1.88248499899827
H	5.18406496570754	3.99839998738254	-1.92397099279550
P	5.82018376443474	-0.96248517901182	-1.90335972948480
P	-1.84859419583772	4.62882950616850	2.22355819259325
P	-1.92180909157088	-1.11830819604815	1.88827984808218
P	-1.94604016713803	-6.24417662991634	2.10821753639059
H	-1.26736699018745	9.64520400142636	2.00846299833780
H	5.18546297216847	4.19249398856874	1.96395597781458
P	5.91373739181472	-0.78427086044380	2.20757549605159
H	0.03440201137745	-8.72777698708604	-3.27856301281084
H	0.03445199792477	7.58455500222896	-3.20734099810993
H	0.03443300876948	2.14545401917398	-3.23346497690212
H	0.03441198982354	-3.29794404035015	-3.26543396415699
H	-3.81718101702750	2.14017400172862	-3.23817000652460
H	-3.81719499569027	-3.29399598765144	-3.25725192336723
H	3.88603901651227	2.14017300361605	-3.24351100033031
H	3.88602501176419	-3.29399600076876	-3.26259197525351
H	-5.11337398050209	3.99839898293964	-1.91683200277587
P	-5.75353835032124	-0.95897128877823	-1.89410353299306
P	1.95497210707214	4.46563990796093	-1.88439766691368
P	1.98586409566925	-0.95788025523655	-1.90753493537326
P	1.96832300983248	-6.41018309291866	-1.93875535379550
H	1.35154400040972	9.45881399964324	-1.88431099989008
H	-7.02727597659739	1.21824100145952	0.00914999597353
H	7.10063291516886	1.21823993218793	-0.00064699230615
P	0.03476149521290	-9.18977153296937	-0.01731288222836
P	0.03715301795568	7.22523898484726	0.01477403335707
P	0.04028446715347	1.75662178221219	0.00658580453873
P	0.04622739708390	-3.65617640895067	-0.02793198674793
H	-3.18266700918557	6.67007200223540	0.04318400114232
P	-3.80187879514166	1.76540620002603	0.02204340023433
P	-3.87430811259599	-3.68520285104511	-0.02544226612896
H	3.25607696604401	6.67007197741503	0.03872000722878
P	3.86698857521765	1.77927684341891	-0.00468243518468
P	3.93756758044341	-3.69240346130930	-0.00711261234673

H	-5.10938393779735	4.19249397128854	1.97109297679457
P	-5.83640072948297	-0.79020801353435	2.22665238823018
P	1.92881483336195	4.62697732495973	2.21522106065035
P	2.05001929248344	-0.81382351354873	2.13516962821908
P	2.01740365729015	-6.25179818548955	2.11263004982123
H	1.34349999250207	9.64520400248541	2.00665300179892
O	-3.98018292085750	-3.66787284354549	3.40338652054557
H	-1.95987572749341	-0.24867976492861	2.99513364372782
H	-4.79683763624387	-3.79515087320737	3.91498883749354
C	1.54113444980122	-4.43811819038075	5.36413593657859
C	1.44619715025029	-3.70777607980419	4.18797801396972
C	-0.87758970519670	-3.71025248497616	4.29373981508421
C	-0.86246530264495	-4.45031107652956	5.46675342883750
C	0.36752053529834	-4.82342282848024	6.01220305044861
H	0.41077569610439	-5.40027875719733	6.92898458216353
H	-1.79773341138474	-4.72618215672182	5.93818616004706
H	-1.80279057723597	-3.36969259700458	3.85344828502055
H	2.32942990987012	-3.38731192223974	3.65116340995051
H	2.51592491428566	-4.70780745234504	5.75083811537262
N	0.25758273599323	-3.34964850646464	3.65790250313854
H	-3.62381576958766	-4.55488338477553	3.19963591171833

Adsorbed Py+H₂O

Energy=-8590.55677336182

H	-1.89126800163321	5.22936299205541	-3.08239699505088
H	-1.89129303185287	-0.21736691925887	-3.11949105632888
H	-1.89131801654660	-5.66540501764425	-3.15456001202736
H	5.81192802034529	-0.21877900668414	-3.12273900734081
H	-1.10798496716707	-10.03481499623220	-0.05366497742113
Ga	-1.86401311182483	5.86323547026363	0.09811514355129
Ga	-1.89690273179486	0.37194633577713	0.14055664902374
Ga	-1.90929876447390	-4.98959161559804	0.07271425841398
Ga	5.79261208747500	0.44043709710067	0.13616565423117
H	5.03736899882503	-4.59106699238545	-0.02090001400504
H	-5.74290197723003	-0.21877800069778	-3.11472598800795
H	1.96034200913831	5.22936299377365	-3.08506698956679
H	1.96031699903866	-0.21736795999286	-3.12215995656912
H	1.96029198898314	-5.66540400319115	-3.15723100031100
H	-6.89107801051949	-1.81628997073326	-1.95500299948045
H	6.96171099914899	-1.81629198634020	-1.96460700823428
Ga	0.02809811338393	3.08833588981131	-2.00800148951773
Ga	0.03021759313867	-2.33987736373857	-2.03071528273217
Ga	0.03618881267524	-7.84003632727025	-2.04144247534819
Ga	0.03521964427160	8.58565970839016	-2.00072458954242
Ga	-3.84135049410513	3.09174186916506	-2.00486962532521
Ga	-3.84030569085687	-2.36188091586542	-2.03592152024915
H	-3.03830899776571	-7.26236999682515	-1.99458000328536
Ga	3.90885600673604	3.10486091838969	-2.02253665371703
Ga	3.90147283530955	-2.36501079687410	-2.03952655163298

H	3.10889200607938	-7.26237200723926	-1.99884199640301
Ga	-5.72147464670584	0.41988143857105	0.17485406159060
H	-4.96404292440386	-4.59106696784518	-0.01396705524009
H	1.18125896152211	-10.03481398512881	-0.05525200673252
Ga	1.93574664238531	5.86487162191488	0.09244968633198
Ga	1.95684153554324	0.42262345659355	0.09050741374869
Ga	1.96040417119545	-5.01071704549354	0.08919684605593
H	-6.91692898133335	-1.58514992686549	1.75643505404699
H	6.99270999643222	-1.58515199688623	1.74679199521737
Ga	0.03494910444805	3.40427424990088	1.63886216651939
Ga	0.06425675983309	-2.14159273293822	1.87333902667526
Ga	0.04156169465911	-7.47200646538064	1.67854146402150
Ga	0.03777864051455	8.93246547117759	1.55702917604474
Ga	-3.75560988963133	3.46697868498210	1.60387397890126
Ga	-3.90643087412803	-2.15311941305406	1.83067053260456
H	-3.06396401756215	-7.03126002791730	1.71723300712769
Ga	3.82920133094903	3.47646086131944	1.59629300156773
Ga	3.98691927893245	-1.99896074333461	1.65723678859114
H	3.13969400805482	-7.03126100233517	1.71293200354189
P	-1.88589276770664	4.46187004379638	-1.88294536422527
P	-1.90874011890537	-0.96003844161837	-1.90195529479684
P	-1.89736150129708	-6.40649077085799	-1.93234311429979
H	-1.28080399830341	9.45881399831415	-1.88248499903263
H	5.18406496167282	3.99839996676643	-1.92397101731378
P	5.81587778840793	-0.96588989251828	-1.90447140700656
P	-1.85245891758521	4.62024443320427	2.21729996811364
P	-1.92612351398691	-0.90203663963113	2.15270510682492
P	-1.94828700107370	-6.23850777150921	2.10429232240464
H	-1.26736699279412	9.64520400401447	2.00846300002243
H	5.18546299386719	4.19249399532274	1.96395598647007
P	5.90234782306828	-0.79159601377745	2.19937430584384
H	0.03440201451168	-8.72777699079220	-3.27856301127385
H	0.03445199658867	7.58455500100624	-3.20734099967028
H	0.03443299360458	2.14545397132867	-3.23346503387926
H	0.03441199941524	-3.29794402800852	-3.26543394119901
H	-3.81718098808197	2.14017397665115	-3.23817001940380
H	-3.81719498531846	-3.29399606744030	-3.25725201490515
H	3.88603902029182	2.14017303282192	-3.24351096032612
H	3.88602500946941	-3.29399600689156	-3.26259198377955
H	-5.11337399895102	3.99839900405492	-1.91683198043780
P	-5.74828663103400	-0.96134362968267	-1.89316161228962
P	1.94890258678264	4.46081117274651	-1.88641483715215
P	1.97350341674546	-0.95860214768788	-1.90735898426434
P	1.96956994908793	-6.40563549554185	-1.93417331908824
H	1.35154400094568	9.45881399977716	-1.88431099904017
H	-7.02727606284922	1.21824096561756	0.00914998832673
H	7.10063295269665	1.21823997111696	-0.00064700213873
P	0.03449177663701	-9.18780455131376	-0.01914768309275
P	0.03570208405968	7.22112594619470	0.01538548593227

P	0.02033288595499	1.74641502562899	-0.00008316823411
P	0.03786586650007	-3.64224091330754	-0.01156158248330
H	-3.18266701186534	6.67007200754734	0.04318400229413
P	-3.78828373483851	1.75681980205226	0.01257682057473
P	-3.87574210770163	-3.67506876488578	-0.01906408563188
H	3.25607699985063	6.67007199861869	0.03872000606733
P	3.86325445956601	1.77680530772421	-0.00711920276032
P	3.93428102755188	-3.69583924272672	-0.00896539249684
H	-5.10938394828342	4.19249397925683	1.97109298412251
P	-5.80893556308460	-0.81523375379577	2.20918430320194
P	1.92444043086081	4.62019809888191	2.21294905439316
P	2.01638795643224	-0.83219528918583	2.11550363620005
P	2.01658392048473	-6.25489110858577	2.11456577534238
H	1.34349999423313	9.64520400368477	2.00665300325467
O	-3.90144749885942	-3.65460852348526	3.36500686197861
H	-4.76515629209550	-3.90684774489633	3.72980188372049
C	1.56929798733648	-4.40260829164543	5.32595910571377
C	1.42836918057990	-3.69388367096664	4.13941877795785
C	-0.87758565149787	-3.60369501497742	4.38346866336161
C	-0.82166236892411	-4.32457719145532	5.56799079082039
C	0.42418180099603	-4.73242006509791	6.04977079883947
H	0.50164248984846	-5.29234487953275	6.97506726387694
H	-1.73702522115564	-4.55666832007625	6.09886353197565
H	-1.81251350685436	-3.22821831327747	3.99386586187911
H	2.28847734586083	-3.42120714433755	3.54272959618110
H	2.55583570464788	-4.69917705204403	5.66054674656116
N	0.22789855725629	-3.30106545097468	3.67130594306693
H	-3.42344121471909	-4.48674146326627	3.16882504550502

5) OH⁻ adsorption effect

Co-adsorbed H₁⁺* and OH⁻

Energy=-8342.36772891477

H	5.77741508875444	18.48719917901272	2.80454890938399
H	5.77741496549618	13.04046334572591	2.76833022399434
H	5.77741481987338	7.59241995060599	2.73413674357229
H	13.48063504568588	13.03905259274582	2.77042345045092
H	6.55859730758932	3.22350849147792	5.83627542594052
Ga	5.80549860575989	19.13001803327676	5.98189387018241
Ga	5.79639111132960	13.70346577081372	5.89790413845581
Ga	5.79562009217405	8.24644517956717	5.99812052731366
Ga	13.46160452292857	13.69489090191355	6.03640209872134
H	12.70392634182968	8.66726167414141	5.87242506504259
H	1.92580498517605	13.03905184601351	2.77042453204108
H	9.62902520068210	18.48719932888301	2.80454878736883
H	9.62902502696660	13.04046306921371	2.76833073652860
H	9.62902487684732	7.59242098600236	2.73413539365619
H	0.77682473070566	11.44172599484778	3.92960758203363
H	14.62961389128911	11.44172600886314	3.92960799052768
Ga	7.71085333943417	16.36192105601728	3.86687990854369

Ga	7.72887284985562	10.91971044534600	3.84639596532799
Ga	7.69645703052190	5.41479275692470	3.85063750338110
Ga	7.70322785646613	21.84620810067660	3.88398835618763
Ga	3.82923749756541	16.36374215181187	3.86745107610158
Ga	3.82129071504466	10.89301959535183	3.84509621609762
H	4.62962040713033	5.99564067730443	3.89357727716950
Ga	11.58094334932972	16.35686671649508	3.87194337665688
Ga	11.58319455669102	10.88758922240015	3.85640651812200
H	10.77682049316151	5.99563923824070	3.89357707659456
Ga	1.94225433597604	13.69111099240533	6.02414493234300
H	2.70251341715411	8.66726131596875	5.87242544992380
H	8.84784140941338	3.22350888983174	5.83627573587261
Ga	9.60328459002482	19.12744922729889	5.98429324476515
Ga	9.62812765736679	13.65059700269802	6.00112505466929
Ga	9.63636065305896	8.24275619547694	5.95341005648586
H	0.74840069035971	11.67346251068246	7.64098899098462
H	14.65803969414588	11.67346264531854	7.64098962146132
Ga	7.70803124021253	16.68182754782400	7.53823380293972
Ga	7.90080763817223	10.89119189644911	7.88451697878037
Ga	7.69408392308043	5.77612797613766	7.56443462726504
Ga	7.70322897052622	22.19324823101268	7.44628230053246
Ga	3.91548524751525	16.74369516050245	7.49867708970413
Ga	3.64067019541807	11.17041444404190	7.58206308196013
H	4.60139089483006	6.22734726257691	7.60533346667467
Ga	11.49774268803110	16.73080063472661	7.48961867348577
Ga	11.66383763492923	11.24734542673352	7.58812979810955
H	10.80504966632178	6.22734637346761	7.60533302047803
P	5.78774664940911	17.72151267032836	4.00510423553995
P	5.76846810088417	12.27988144532188	3.96604753701838
P	5.76716917086337	6.85613852146959	3.96117768504779
H	6.38704564149138	22.71684346250759	4.00420320420028
H	12.85194063486106	17.25642356018889	3.96807754350702
P	13.48673309345668	12.29471083839179	3.99042459420198
P	5.81691727802677	17.88752279063877	8.11040325196619
P	5.79210643021598	12.15711044611457	7.77528668455594
P	5.72164254911976	7.01072182822539	8.02289764920724
H	6.39778582406350	22.90385778416257	7.89512879029588
H	12.85064304594474	17.45114201232735	7.85597217711037
P	13.57616506355271	12.46997666296875	8.10181306692615
H	7.70321980976495	4.53002830758933	2.61196074489404
H	7.70321992809139	20.84237170629751	2.68056183518092
H	7.70322005718578	15.40326648154827	2.65531097458269
H	7.70321995199491	9.95986308065536	2.62421706751985
H	3.85161012450923	15.39798390009655	2.64793611436390
H	3.85160999379868	9.96381130325950	2.62972778269360
H	11.55483003798840	15.39798440890950	2.64793744406439
H	11.55482990260734	9.96381192413139	2.62972868293838
H	2.55450142818985	17.25642184670300	3.96807771332131
P	1.91930408978435	12.29345906792173	3.98795408489426

P	9.62624353606993	17.72384382268453	4.00492061082354
P	9.65392918100279	12.30116244579976	3.98377611784745
P	9.63456809567501	6.84586362216795	3.95122746439040
H	9.01939446452298	22.71684275562713	4.00420263269110
H	0.63926635437493	14.47657194786911	5.89317727742476
H	14.76717417963706	14.47657325446606	5.89317637370729
P	7.70255651212045	4.06757677365369	5.87020741664789
P	7.70449981801954	20.48246127197251	5.90314687714409
P	7.71911509188669	15.02383762327167	5.89088115611206
P	7.71526103546354	9.62229089107575	5.85012036600542
H	4.48384905928326	19.92840923967326	5.92900073770841
P	3.87706537567640	15.02449087903146	5.90489128515376
P	3.80559219051648	9.55540132572858	5.87256306134941
H	10.92259262260978	19.92841058371257	5.92900143122790
P	11.52495929129525	15.02489552444584	5.89154568127337
P	11.60522729630207	9.56821285006407	5.89186973764285
H	2.55579653077041	17.45114115188277	7.85597173736446
P	1.81677194751870	12.48480448408676	8.11281264301709
P	9.59822549949891	17.88602705958445	8.10615383173885
P	9.68681472932908	12.41771189401614	8.03940158083570
P	9.67107673799325	7.00973377648582	7.98438359405938
H	9.00865308275566	22.90385830903231	7.89512909766159
O	7.76325681545906	9.77561704027809	9.38341866557043
H	8.29904270225569	8.97364424284628	9.27964567482398
H	5.65056016188953	13.04472231561425	8.85964364336467

Adsorbed OH⁻

Energy=-8341.9071463323

H	5.77741509150618	18.48719916848657	2.80454891813959
H	5.77741499522131	13.04046332442422	2.76833026937254
H	5.77741498737688	7.59242013790988	2.73413662793208
H	13.48063500489401	13.03905264071108	2.77042342083639
H	6.55859728063327	3.22350848053045	5.83627540133228
Ga	5.80254495738690	19.12078780397812	5.98383718889075
Ga	5.79530612249476	13.64682323314160	6.02003128849979
Ga	5.78748493187530	8.26829128631629	5.99129411055009
Ga	13.45780214864024	13.69575572115881	6.03615859229306
H	12.70392617377714	8.66726174738548	5.87242506276248
H	1.92580501844169	13.03905188133569	2.77042450626019
H	9.62902520975052	18.48719932874792	2.80454879078426
H	9.62902500866396	13.04046302605977	2.76833077972060
H	9.62902483027719	7.59242108370581	2.73413533101535
H	0.77682468015480	11.44172596124504	3.92960760375125
H	14.62961395400097	11.44172596018935	3.92960800537623
Ga	7.70235363120654	16.34781905445632	3.87918226053621
Ga	7.70337582153139	10.91883367205945	3.85432600821553
Ga	7.69850710304921	5.42235121559002	3.84790335887866
Ga	7.70319639211544	21.84263625255954	3.88828540996222
Ga	3.82859020534519	16.35297952504301	3.87848059325917

Ga	3.84066309725822	10.88958420619864	3.85906967118411
H	4.62962020805524	5.99564049647449	3.89357731757857
Ga	11.57801368128555	16.35572551936562	3.87556331504278
Ga	11.56712325155599	10.88953806605767	3.85882291609197
H	10.77682058932355	5.99563914826309	3.89357709097665
Ga	1.94865142666338	13.69442194621376	6.03754331451061
H	2.70251345250017	8.66726135626756	5.87242544637155
H	8.84784144143337	3.22350887478821	5.83627573936689
Ga	9.60370317524131	19.12113603158913	5.98341398423666
Ga	9.61752712777704	13.65378426893593	6.00775633384885
Ga	9.61824084217992	8.26489239979644	5.96769692236443
H	0.74840072881626	11.67346253000093	7.64098898013152
H	14.65803959018729	11.67346271407540	7.64098963161654
Ga	7.70383218855441	16.66740171684631	7.53068853729238
Ga	7.71059429847158	10.99372309136438	7.86316131132928
Ga	7.69116171478991	5.78432052095611	7.56164309109929
Ga	7.70324232481100	22.18962742364833	7.44550829554305
Ga	3.90984171525253	16.72557359033978	7.48877044478186
Ga	3.77693083770074	11.24705758307632	7.58680455634730
H	4.60139103031223	6.22734733816365	7.60533348659058
Ga	11.49684245304015	16.72691544331098	7.48665235047336
Ga	11.63150553170290	11.25316921798018	7.58070735753582
H	10.80504963888018	6.22734636454944	7.60533302997259
P	5.78506906446390	17.71940155314604	4.00336780574010
P	5.76541513919713	12.30159519849177	3.98621107419856
P	5.76596375098390	6.85787202596733	3.96282857122059
H	6.38704563503588	22.71684348616824	4.00420321005398
H	12.85194062557005	17.25642358701261	3.96807759328704
P	13.48255022916306	12.29151066997278	3.98939008636094
P	5.81209931000232	17.87964629204022	8.10500639294621
P	5.76721828024478	12.38027505633663	8.03604370186737
P	5.72080117273845	7.01530764747048	8.01668704263892
H	6.39778564048996	22.90385777932643	7.89512883740167
H	12.85064304339753	17.45114201516745	7.85597218336541
P	13.56417621234155	12.46222657167010	8.09484194363332
H	7.70321978654928	4.53002828620879	2.61196080244787
H	7.70321988129680	20.84237162431624	2.68056173875690
H	7.70322004939004	15.40326645732881	2.65531097097345
H	7.70321995004347	9.95986310399803	2.62421708314219
H	3.85161009953342	15.39798393046769	2.64793611991350
H	3.85160997402089	9.96381128219406	2.62972776964696
H	11.55483003065046	15.39798435676849	2.64793740353594
H	11.55482992857506	9.96381189706746	2.62972864955099
H	2.55450147019113	17.25642181088775	3.96807770373347
P	1.92422546196687	12.29123995469529	3.98942510284765
P	9.62049245177611	17.71936041248754	4.00316063645633
P	9.64204210338993	12.30100320302427	3.98419762432572
P	9.63690069497982	6.85211999371259	3.95711963837758
H	9.01939453695537	22.71684280068327	4.00420265279377

H	0.63926637784478	14.47657189629918	5.89317728099181
H	14.76717422545944	14.47657322202751	5.89317635024269
P	7.70260295404929	4.06947156134269	5.86803604509038
P	7.70307666355574	20.47828764487635	5.90405002660361
P	7.70382031029592	15.01541902939956	5.88697761589518
P	7.70437243775965	9.63490480127901	5.85942879237127
H	4.48384906689149	19.92840922616003	5.92900074371769
P	3.88815407419540	15.01795585090612	5.89391928982783
P	3.80302468952718	9.56693554886726	5.89125186521891
H	10.92259261623999	19.92841057597977	5.92900143698922
P	11.52222194387317	15.02365692011689	5.88848397780370
P	11.60264869497200	9.56596073574790	5.89065350273145
H	2.55579653933057	17.45114115165408	7.85597173237697
P	1.84347705060892	12.46096963624653	8.09571354700652
P	9.59494158727360	17.88028882131702	8.10490543758027
P	9.64861528574162	12.39613225724183	8.01831122749005
P	9.67111672864220	7.00899056956473	7.98973961408701
H	9.00865325206131	22.90385836440983	7.89512912347291
O	7.69505887118994	9.83534972916917	9.36090244725120
H	8.27794861038317	9.07363025852509	9.21923404555273

6) HCOO⁻ adsorption effect

Co-adsorbed H₁⁺* and HCOO⁻

Energy=-8455.67694283767

H	5.77741497955396	18.48719902145108	2.80454897610604
H	5.77741498535072	13.04046299651038	2.76833002124540
H	5.77741496172667	7.59241994568042	2.73413700626493
H	13.48063511828968	13.03905291686145	2.77042303980480
H	6.55859697410083	3.22350902672426	5.83627500821516
Ga	5.80612328466323	19.13098776259737	5.97849395200458
Ga	5.77225119448541	13.83451289636785	5.77420198276734
Ga	5.75118726268717	8.22581726388883	5.98332868299995
Ga	13.45985338468055	13.69182121369091	6.04258825151671
H	12.70392599645914	8.66726199928543	5.87242502368110
H	1.92580490335809	13.03905192424715	2.77042503743014
H	9.62902499875317	18.48719900254326	2.80454902316156
H	9.62902502386379	13.04046301460368	2.76833098032804
H	9.62902501737181	7.59242094595865	2.73413502916409
H	0.77682507955134	11.44172607633663	3.92960794991815
H	14.62961387499945	11.44172611589168	3.92960796688550
Ga	7.73185883811298	16.38200857354702	3.84959931639694
Ga	7.71842994455728	10.92316883889374	3.84829211852602
Ga	7.70359651626268	5.41557287507745	3.84879229274364
Ga	7.70336393205264	21.84689784344800	3.88304606549132
Ga	3.82361518924781	16.38048224284083	3.84923253788599
Ga	3.80942253728864	10.88143304593551	3.86585186315675
H	4.62962003878584	5.99564104798366	3.89357699042197
Ga	11.58086657156074	16.34802992619062	3.88088488039097
Ga	11.57946483966313	10.89112806237016	3.85372226019365

H	10.77682095776493	5.99563903964983	3.89357698040385
Ga	1.94018953310374	13.65913567388496	6.06822491019506
H	2.70251300251453	8.66726100714160	5.87242500600948
H	8.84784103823557	3.22350896524749	5.83627599862838
Ga	9.60307269538057	19.13061813228274	5.98978013366376
Ga	9.60453354995378	13.63185509024601	6.03815898094971
Ga	9.63468396281647	8.24263081913627	5.98718896780465
H	0.74840091473930	11.67346295976219	7.64098899373832
H	14.65804006846961	11.67346297806024	7.64098998929181
Ga	7.70590335003501	16.69303080297567	7.53411223209827
Ga	7.67626234098168	11.03339095362506	7.73806503088771
Ga	7.70763521278721	5.76450070861666	7.55746533183595
Ga	7.70310746964898	22.19384214321916	7.44597575899939
Ga	3.91393544880027	16.75313394551802	7.48368204645917
Ga	3.76297196339570	11.04846436426072	7.78711462779675
H	4.60139098531686	6.22734700249310	7.60533299546819
Ga	11.49502900774459	16.72966115827642	7.49728361449646
Ga	11.64136862636141	11.21337075033235	7.60093890195468
H	10.80505001830357	6.22734599228443	7.60533300021928
P	5.79214819277286	17.72086151936149	4.00211182100986
P	5.75887532540860	12.28787558532162	3.96005245378335
P	5.76957772764637	6.84887105156773	3.95532417782806
H	6.38704602681834	22.71684298112525	4.00420298748139
H	12.85194102023531	17.25642400722652	3.96807796548300
P	13.48635674832149	12.29494849024991	3.99102758677802
P	5.81386360397405	17.89238678028784	8.11087541752653
P	5.73433529725755	12.38622843688000	7.61545483070293
P	5.73745629030490	6.98267613863957	8.00573307675930
H	6.39778618757488	22.90385801544818	7.89512894650574
H	12.85064291276944	17.45114198031358	7.85597197043971
P	13.55894931395456	12.45622652504616	8.09926485259210
H	7.70322001545925	4.53002804482194	2.61196099936493
H	7.70322005857535	20.84237209858323	2.68056210222153
H	7.70322000048727	15.40326603994098	2.65531102795517
H	7.70321999955399	9.95986297760216	2.62421698225728
H	3.85160999206849	15.39798401792434	2.64793603340630
H	3.85161000148785	9.96381102806198	2.62972802458297
H	11.55482999609303	15.39798401639404	2.64793703008466
H	11.55482998931460	9.96381203513333	2.62972901825388
H	2.55450098544895	17.25642200342245	3.96807796864861
P	1.91744236758221	12.29693835693632	3.99311800251101
P	9.63727877591790	17.73256730754974	4.00562997234981
P	9.64808703363112	12.30180345270183	3.99054029571267
P	9.63616478203606	6.85172271710759	3.95741849254944
H	9.01939388341171	22.71684293339413	4.00420297157455
H	0.63926611528396	14.47657200452235	5.89317700154468
H	14.76717390629263	14.47657295577716	5.89317599894966
P	7.70447757622480	4.06469101548914	5.86461391998408
P	7.70431238302385	20.48395560384987	5.90215112597090

P	7.73859027555871	15.06035876163523	5.86691933170644
P	7.68381467833388	9.59117114716728	5.84906581581671
H	4.48384906880587	19.92840896718609	5.92900099786056
P	3.82848714793530	15.06999099468691	5.86961172015451
P	3.80167748411254	9.57179124958261	5.89991666211243
H	10.92259298337639	19.92841100056339	5.92900099567180
P	11.51103786537899	15.00694880708251	5.91179964957774
P	11.60107899841928	9.56323722138380	5.88493953052528
H	2.55579805712130	17.45114097656237	7.85597197904918
P	1.86736842837809	12.42446620842269	8.11595558857972
P	9.59803989386188	17.89076183258962	8.11183926307411
P	9.62308006809878	12.33347986600483	8.08745226540334
P	9.67594178462105	7.00304982709539	8.01156113065569
H	9.00865282369689	22.90385794196147	7.89512896731392
O	4.59852014255814	9.98529577307132	9.34263616164247
O	6.90718560927290	9.94122357226276	9.29870316146740
C	5.75508104508509	9.68894046322849	9.78093203941859
H	5.76374323480954	9.13558898324087	10.72778562898547
H	5.73465123445236	13.19316269579865	8.76927649037164

Adsorbed HCOO⁻

Energy=-8455.21594752846

H	5.77741497279906	18.48719902414440	2.80454898443683
H	5.77741497762034	13.04046301600748	2.76833001137154
H	5.77741496184554	7.59241994507081	2.73413700326203
H	13.48063512322697	13.03905292018840	2.77042303725710
H	6.55859697640160	3.22350902161804	5.83627500865987
Ga	5.80320483340333	19.12198333952955	5.98098955005406
Ga	5.76210854790502	13.73635756398188	5.91543716972568
Ga	5.74796238185367	8.25231644344476	5.98710242673982
Ga	13.45667510880727	13.69422158231082	6.04310748181963
H	12.70392600488441	8.66726199527961	5.87242501796922
H	1.92580492109687	13.03905192639330	2.77042504758040
H	9.62902500213309	18.48719900325123	2.80454902771554
H	9.62902502367547	13.04046302020180	2.76833099070944
H	9.62902501251493	7.59242094972358	2.73413502608192
H	0.77682508325005	11.44172608204426	3.92960795427854
H	14.62961387429832	11.44172611458932	3.92960796521654
Ga	7.71966385090108	16.36444820294248	3.86484394358966
Ga	7.69494531535694	10.92069328220399	3.85524447754007
Ga	7.70088612575198	5.42663714147767	3.84296091674363
Ga	7.70327802343712	21.84341514932025	3.88743127238889
Ga	3.82394842420158	16.36755302665126	3.86241834430009
Ga	3.82527326002540	10.87860120883611	3.87398756424337
H	4.62962003552913	5.99564104352067	3.89357698835627
Ga	11.57745454398587	16.34762191549543	3.88450897155526
Ga	11.56666127593523	10.89467867553280	3.85458717639235
H	10.77682096591035	5.99563903245675	3.89357698234924
Ga	1.94658777207104	13.66696845901211	6.07815869248798

H	2.70251301546082	8.66726101042535	5.87242499742226
H	8.84784103477326	3.22350896981263	5.83627599826034
Ga	9.60290459857135	19.12390889251508	5.98849244461738
Ga	9.59282734849018	13.63550798672238	6.04124677545750
Ga	9.61440884275656	8.26645600255128	5.99972138487492
H	0.74840098185936	11.67346298235272	7.64098900373615
H	14.65804007296533	11.67346297655440	7.64098998733808
Ga	7.69845085978496	16.66756588081194	7.52013162778599
Ga	7.52423995735457	11.14279115682798	7.71358325870544
Ga	7.70688339979051	5.76460024030592	7.54653352823091
Ga	7.70309541541040	22.19117863388398	7.44440489587513
Ga	3.90865721507237	16.73330107207714	7.47382726503877
Ga	3.89882721236112	11.15335200514117	7.75981892482631
H	4.60139098858724	6.22734699909890	7.60533299679593
Ga	11.49397092418693	16.72790748456995	7.49244815782712
Ga	11.61846530902361	11.22276632980616	7.58833252426221
H	10.80505001222322	6.22734599431051	7.60533300088968
P	5.78866208139490	17.71925713333061	4.00096295077957
P	5.75447267293184	12.30016404719489	3.97654190664806
P	5.76669562981246	6.85449621239711	3.95989412862939
H	6.38704602901228	22.71684297974378	4.00420298688686
H	12.85194101579011	17.25642400454531	3.96807796373408
P	13.48365164060219	12.29306748052310	3.99064193906483
P	5.81076446084360	17.88149934231401	8.10303035276995
P	5.72880265222979	12.61909434683526	7.94189006391501
P	5.74169855383707	6.97635747749209	7.99763704951806
H	6.39778619042617	22.90385801596145	7.89512894592226
H	12.85064291139677	17.45114198152146	7.85597196934493
P	13.55166822346491	12.45138422468096	8.09356248262428
H	7.70322001587768	4.53002804314250	2.61196099577570
H	7.70322005835020	20.84237210014620	2.68056210427536
H	7.70322000059596	15.40326602766296	2.65531102140745
H	7.70322000045912	9.95986296807425	2.62421699081679
H	3.85160999246980	15.39798401910378	2.64793604832170
H	3.85161000834213	9.96381101124184	2.62972802544051
H	11.55482999820687	15.39798401895645	2.64793703207358
H	11.55482999237180	9.96381203217557	2.62972901990876
H	2.55450099998615	17.25642199456896	3.96807797440673
P	1.92115988928294	12.29548060632677	3.99445689703995
P	9.62931332722734	17.72679591866751	4.00395383612644
P	9.63767759673714	12.30053741389119	3.99002333111311
P	9.63724250564824	6.85760541323120	3.96254247257691
H	9.01939388217402	22.71684293307203	4.00420297110360
H	0.63926599604984	14.47657202621691	5.89317697340454
H	14.76717389122320	14.47657294737354	5.89317599986915
P	7.70483638998461	4.06469708098710	5.85736723089281
P	7.70280206825842	20.48061145122625	5.90279849116050
P	7.71175540209565	15.03884453175942	5.85867692274390
P	7.67229360901885	9.61920779891608	5.86313016331074

H	4.48384906566273	19.92840897126186	5.92900099564355
P	3.84504202735753	15.05553154708831	5.85988635950914
P	3.79933142800099	9.58530005760221	5.90679970823057
H	10.92259297657496	19.92841099753772	5.92900099587975
P	11.50859967511495	15.00650694082925	5.90806214845385
P	11.59883382195943	9.56104580665346	5.88283627838021
H	2.55579807496818	17.45114096452899	7.85597196934933
P	1.88718614650788	12.40686221509207	8.10115268081274
P	9.58973820179531	17.87962514584333	8.10623102450609
P	9.59609594228217	12.31787655263972	8.06852810065270
P	9.67399816182402	7.00002410140426	8.01218824635236
H	9.00865282039107	22.90385794080182	7.89512896649240
O	4.59293313748887	9.91974899930390	9.29771672224848
O	6.89724920905011	9.88591067625642	9.24838507272483
C	5.74983203050408	9.62135523275446	9.73341354443577
H	5.76260709136204	9.05248850501839	10.67251623944397

7) H₂O+OH⁻ adsorption effect

Co-adsorbed H₁⁺* and H₂O+OH⁻

Energy=-8418.80540026295

H	-1.89126799901149	5.22936299793697	-3.08239700025302
H	-1.89129304034937	-0.21736701799186	-3.11949099033000
H	-1.89131802445038	-5.66540501222636	-3.15456000333634
H	5.81192801756389	-0.21877900763145	-3.12273899742760
H	-1.10798497346849	-10.03481499938603	-0.05366498437753
Ga	-1.86117238942657	5.87036515655365	0.09165421991822
Ga	-1.89564571990783	0.52290066893741	-0.06624238997598
Ga	-1.93216787974256	-5.00920520821975	0.09551619044415
Ga	5.79378658181553	0.43399657108441	0.14907158541035
H	5.03736900015177	-4.59106700596342	-0.02090000729960
H	-5.74290198098786	-0.21877800111923	-3.11472598329045
H	1.96034200357568	5.22936299294023	-3.08506699694072
H	1.96031700123928	-0.21736799653083	-3.12215999537200
H	1.96029199876923	-5.66540400614577	-3.15723099579318
H	-6.89107801999327	-1.81628999652390	-1.95500299993357
H	6.96171098522361	-1.81629198640199	-1.96460700490365
Ga	0.05472910439149	3.11336384647771	-2.02936834880199
Ga	0.04682247238971	-2.33199762153978	-2.04645858978789
Ga	0.02806592130584	-7.83875948524351	-2.04442489687397
Ga	0.03536485337232	8.58814189802593	-2.00374981262616
Ga	-3.84415286641621	3.11251682686942	-2.02632205119126
Ga	-3.85995019110080	-2.38372779657771	-2.01379299407097
H	-3.03830899921546	-7.26237000320226	-1.99458001208695
Ga	3.91173024402625	3.09270974886819	-2.01231482575423
Ga	3.91129727014196	-2.36569457200926	-2.03955061335046
H	3.10889199502511	-7.26237199314658	-1.99884199665471
Ga	-5.72706024029556	0.39765788458857	0.18142921649283
H	-4.96404284125257	-4.59106687061272	-0.01396703363168
H	1.18125897135636	-10.03481398567055	-0.05525200053365

Ga	1.93644500152022	5.87045230348729	0.09788674068903
Ga	1.94432215419123	0.38082264328467	0.13954607141863
Ga	1.96998325865702	-5.01915511396587	0.07965570736916
H	-6.91692904968954	-1.58514998963424	1.75643501579503
H	6.99270999711183	-1.58515199323382	1.74679199570035
Ga	0.03907277153387	3.42768487641700	1.64409953689680
Ga	0.06022720246093	-2.23303617078571	1.83195245646701
Ga	0.03495906904750	-7.49488454618280	1.64884941276996
Ga	0.03762667399679	8.93461931589938	1.55808631873515
Ga	-3.75284676508431	3.48821476144284	1.59847701683748
Ga	-3.97093801499231	-2.28471543293081	1.99719280842146
H	-3.06396403479936	-7.03126003928396	1.71723300140755
Ga	3.82940364119910	3.47210315870743	1.60560858525776
Ga	3.98524414798212	-2.04455242559082	1.70268568140408
H	3.13969401204545	-7.03126100336519	1.71293200355476
P	-1.87857052702016	4.46171173300556	-1.88450043388240
P	-1.91190690811423	-0.97432040589910	-1.92748244785853
P	-1.90237641954799	-6.40275887754489	-1.92932170656121
H	-1.28080399746502	9.45881399904281	-1.88248499867996
H	5.18406498957878	3.99839999486520	-1.92397099750727
P	5.81864229402775	-0.96290613910725	-1.90236847697655
P	-1.85165103301295	4.63005671544108	2.22222460931390
P	-1.94421571830876	-0.95483214060887	1.76634276228660
P	-1.92542403831606	-6.26893765757311	2.11076957970204
H	-1.26736699644934	9.64520400330727	2.00846299984494
H	5.18546299367120	4.19249400041954	1.96395599617090
P	5.89719501784828	-0.80110505816167	2.20655744530864
H	0.03440201015902	-8.72777699213631	-3.27856300186395
H	0.03445199880034	7.58455500106811	-3.20734100038055
H	0.03443300049421	2.14545400273304	-3.23346499443123
H	0.03441200032257	-3.29794402089066	-3.26543401768457
H	-3.81718100017248	2.14017400287263	-3.23817000126312
H	-3.81719499341634	-3.29399602559669	-3.25725198802511
H	3.88603900443741	2.14017300527374	-3.24351099323074
H	3.88602500285778	-3.29399599980811	-3.26259199927586
H	-5.11337399445631	3.99839899628825	-1.91683199668820
P	-5.74925892145766	-0.96200093111807	-1.89339968223574
P	1.96394218919876	4.47046695465988	-1.88449344010759
P	1.98010055260457	-0.95660407101383	-1.90129203434451
P	1.96692913662325	-6.41023783523196	-1.93805920068125
H	1.35154399955490	9.45881399874000	-1.88431100011212
H	-7.02727601673291	1.21824098322460	0.00914999437823
H	7.10063296625186	1.21823997838749	-0.00064699551818
P	0.03757514453128	-9.19502643839633	-0.03283733104013
P	0.03731760916211	7.22447188427847	0.01460964322093
P	0.05942000667803	1.78408701820380	-0.01304602020851
P	0.02466138184639	-3.67163233951309	-0.05681914481067
H	-3.18266700638631	6.67007200213207	0.04318399912758
P	-3.82631197389415	1.79512101718136	-0.00732781742954

P	-3.88310010355247	-3.66852341364411	0.02482200157675
H	3.25607699239005	6.67007199564361	0.03872000168570
P	3.84862420776594	1.75327089509486	0.01692738413109
P	3.93508859729755	-3.69546690560947	-0.00969306418098
H	-5.10938396706729	4.19249398962208	1.97109298538332
P	-5.80986382614883	-0.81799159535422	2.22232798317656
P	1.93056877186271	4.62933752369280	2.21948299961905
P	1.97973119337500	-0.91359550023582	2.19096609595357
P	2.00335981031087	-6.25570514267224	2.10593690041902
H	1.34349999645406	9.64520400110624	2.00665300115597
O	-3.28994959882798	-3.39831897152222	3.42067752349912
O	-0.71906895959820	-3.37011245393430	3.38513794986051
H	-1.90000138859368	-0.11763768068155	2.89888786963533
H	-3.55937864826182	-3.04926342076556	4.28518176178919
H	-1.76508888775130	-3.42229289860848	3.40998678736113
H	-0.36791198664062	-4.25838291460128	3.55532962886219

Adsorbed H₂O+OH⁻

Energy=-8418.33894008625

H	5.77741507805338	18.48719918994189	2.80454893309095
H	5.77741488965237	13.04046332053683	2.76833024403240
H	5.77741490163875	7.59242005726281	2.73413664756212
H	13.48063524068133	13.03905249579488	2.77042348967508
H	6.55859728250576	3.22350850325964	5.83627544024733
Ga	5.80246547414623	19.12040662506480	5.98172436017318
Ga	5.75599662695585	13.69984418513645	5.94952022749375
Ga	5.73181654776568	8.27376302740760	5.98249605410118
Ga	13.45674381767187	13.69532219369747	6.04262126631036
H	12.70392627945885	8.66726175194360	5.87242510998989
H	1.92580487033090	13.03905174580388	2.77042460457405
H	9.62902516852102	18.48719932139144	2.80454883486225
H	9.62902505330035	13.04046303561584	2.76833078989530
H	9.62902483635024	7.59242103620336	2.73413537040242
H	0.77682479863239	11.44172609131711	3.92960749215337
H	14.62961374785669	11.44172615876519	3.92960795217213
Ga	7.71352651716753	16.35582711905100	3.87264221813619
Ga	7.69060862862783	10.92520627643112	3.84993647022379
Ga	7.69422553780052	5.42992326738551	3.83963275925895
Ga	7.70319690228223	21.84295823593549	3.88802223908081
Ga	3.82399303139966	16.36085901892217	3.86975766731323
Ga	3.82304381125836	10.87413196589082	3.87842926537549
H	4.62962028746962	5.99564056617097	3.89357729990235
Ga	11.57667081335527	16.34989173137383	3.88287856401584
Ga	11.56716374358424	10.89584458327719	3.85356693531169
H	10.77682054149343	5.99563919467311	3.89357707579574
Ga	1.94548066774034	13.66370828795601	6.07710911168102
H	2.70251354121694	8.66726146115065	5.87242544777899
H	8.84784143612986	3.22350887963851	5.83627573655494
Ga	9.60271320018747	19.12301087193991	5.98679613740330

Ga	9.59673897942766	13.64101885370513	6.03436263279643
Ga	9.61664790678340	8.26173515440633	5.98119035378168
H	0.74840063937880	11.67346247288949	7.64098896726193
H	14.65803976552582	11.67346263161466	7.64098960002608
Ga	7.69750797488025	16.66303345624703	7.51995450325526
Ga	7.57045375083666	11.13453707904620	7.70224789770347
Ga	7.69883952577129	5.76239067180588	7.52890439957412
Ga	7.70310028339387	22.19039263924732	7.44465168906962
Ga	3.90790636152089	16.72917263089947	7.47578080804495
Ga	3.83972436051875	11.08084908814150	7.84935589688941
H	4.60139086039768	6.22734722937130	7.60533348213117
Ga	11.49375178956790	16.72892013843858	7.49199530793350
Ga	11.62682102555450	11.22297089510649	7.58243932143987
H	10.80504968636491	6.22734637160684	7.60533301180229
P	5.78697271682186	17.71833074592966	4.00142396668476
P	5.75059405462491	12.29882471653739	3.97753811418234
P	5.76319043347355	6.85941160693507	3.96271441032201
H	6.38704561553342	22.71684346389989	4.00420321448614
H	12.85194066250951	17.25642361809088	3.96807757390071
P	13.48424848433269	12.29346123288645	3.99046227224132
P	5.81052233874532	17.87983269559538	8.10254754202982
P	5.71687538609826	12.53884872970319	7.95516538604953
P	5.74305648000324	6.98631418223711	7.98940601070801
H	6.39778612827514	22.90385780871561	7.89512871898352
H	12.85064296482345	17.45114199316995	7.85597214159549
P	13.55426136889175	12.45243246997964	8.09360032352106
H	7.70321981403482	4.53002833639724	2.61196081099299
H	7.70322003803033	20.84237178275948	2.68056194037533
H	7.70322006155296	15.40326650847428	2.65531100367092
H	7.70321995311135	9.95986306484850	2.62421701651180
H	3.85161005349129	15.39798402954577	2.64793624153857
H	3.85160999400388	9.96381134290088	2.62972784750427
H	11.55483003391979	15.39798434867958	2.64793738952658
H	11.55482987922017	9.96381199200438	2.62972869416984
H	2.55450150653591	17.25642177294105	3.96807761187645
P	1.92145332161752	12.29508867867853	3.99325862963378
P	9.62539524178194	17.72402711085234	4.00374414872423
P	9.63759463044428	12.30015304794814	3.98865066832925
P	9.63610705292000	6.85327683497642	3.95802623169654
H	9.01939435341790	22.71684268763564	4.00420261224924
H	0.63926654489099	14.47657187044848	5.89317727684279
H	14.76717397238931	14.47657311947741	5.89317635200029
P	7.70439372306058	4.06258839591494	5.85052212253930
P	7.70232686221104	20.47999347682173	5.90294752956115
P	7.70056968013141	15.02444538163737	5.86775519707899
P	7.67967952564478	9.61340106848305	5.84845027255620
H	4.48384900676888	19.92840927006330	5.92900073121512
P	3.85074991525408	15.04463188041249	5.86877127961083
P	3.78198118790732	9.60141891612961	5.91386149265078

H	10.92259263026883	19.92841059702628	5.92900143276263
P	11.51103967335364	15.01041471870743	5.90530362674817
P	11.59924366256373	9.55998721495147	5.88025907833426
H	2.55579671362825	17.45114108449071	7.85597164980046
P	1.87443289200625	12.42264180261289	8.09496866146406
P	9.58814159168744	17.87828688546036	8.10442565179189
P	9.61603629670019	12.32888766424549	8.06361870837617
P	9.66587264716894	6.99909989096266	7.99666968400403
H	9.00865278590895	22.90385820562664	7.89512904166045
O	4.36366579984319	9.80972352840936	9.24604240531333
O	6.92299522157607	9.86315561783922	9.24079846276739
H	4.10441299747973	10.16088141180636	10.11317167949899
H	5.87376630910763	9.80029950623096	9.26092875651947
H	7.26592542320713	8.95826116324367	9.30582676024036

8) Py+OH⁻ adsorption effect

Co-adsorbed H₁⁺* and Py+OH⁻

Energy=-8590.56197960303

H	-1.89126797494699	5.22936299823289	-3.08239700850060
H	-1.89129302850353	-0.21736705654996	-3.11949094877796
H	-1.89131802971843	-5.66540502403433	-3.15455999408150
H	5.81192800398281	-0.21877900383469	-3.12273899823498
H	-1.10798497818262	-10.03481499909450	-0.05366497969412
Ga	-1.86209077011061	5.86848125500523	0.09413421733323
Ga	-1.90188100880028	0.42721400826648	0.02211938332423
Ga	-1.93183277861184	-4.99415336848388	0.11511982071131
Ga	5.79467622199786	0.43853066827898	0.13706516082781
H	5.03736900498613	-4.59106700650346	-0.02090000971874
H	-5.74290198476926	-0.21877802593943	-3.11472595256270
H	1.96034202370066	5.22936300237215	-3.08506702522731
H	1.96031702090332	-0.21736801503831	-3.12216003809245
H	1.96029200341381	-5.66540401104996	-3.15723099666958
H	-6.89107800591696	-1.81628997494303	-1.95500299697978
H	6.96171098786874	-1.81629199161950	-1.96460699357913
Ga	0.03632544672360	3.09805181550777	-2.01628596404789
Ga	0.04480959711681	-2.34174477146025	-2.03473832648946
Ga	0.02438211406767	-7.83798738132344	-2.04156862250615
Ga	0.03524718122913	8.58760108103763	-2.00309992699648
Ga	-3.84189695138569	3.09961115105401	-2.01266787776191
Ga	-3.85898842713923	-2.38603807119384	-2.01476096283068
H	-3.03830899836098	-7.26237000039549	-1.99458001595688
Ga	3.91087580273472	3.10428420779109	-2.02375648823957
Ga	3.90966989520407	-2.36788728653188	-2.03914534012055
H	3.10889198948578	-7.26237198930498	-1.99884199706332
Ga	-5.72908399477495	0.40220898091948	0.16016667279421
H	-4.96404284737700	-4.59106686067017	-0.01396702093574
H	1.18125897112094	-10.03481398243125	-0.05525200069552
Ga	1.93583398799819	5.86860564974758	0.09400224252064
Ga	1.96309462611042	0.41448937136489	0.09166414029357

Ga	1.96719949034516	-5.02501563107854	0.08740333073312
H	-6.91692914333021	-1.58515001948872	1.75643497029805
H	6.99271002949175	-1.58515201097612	1.74679200621344
Ga	0.03648328248331	3.41556890049697	1.64275202032508
Ga	0.17070964091503	-2.21374885588982	1.87404254516590
Ga	0.02891097375911	-7.47873884672529	1.65509671407932
Ga	0.03770633277490	8.93407123576642	1.55818793067914
Ga	-3.75356218744686	3.47965524370854	1.60540961823601
Ga	-4.08837711877834	-2.34249769200052	2.02995495412545
H	-3.06396403672111	-7.03126004114987	1.71723299658630
Ga	3.83065808986636	3.47646668979001	1.59815196768769
Ga	4.00637123763373	-2.00911004961859	1.66685362873686
H	3.13969401255357	-7.03126099988964	1.71293200066704
P	-1.88356208789153	4.46224662366305	-1.88285658962994
P	-1.91217828122722	-0.98201392920342	-1.92205487639674
P	-1.90437099961986	-6.39564237038569	-1.92362485085006
H	-1.28080400242933	9.45881400192260	-1.88248499928894
H	5.18406499733603	3.99839999942596	-1.92397100137116
P	5.81767556910613	-0.96473855388089	-1.90412722065520
P	-1.85083919994719	4.62473423497106	2.22153940686329
P	-1.94827154667541	-1.10488715364932	1.88539676090659
P	-1.93793036388469	-6.25883215210808	2.12597063697983
H	-1.26736699475469	9.64520400319500	2.00846299981081
H	5.18546299211668	4.19249400634325	1.96395600286917
P	5.90891514534623	-0.78829990578993	2.20489623086658
H	0.03440201493429	-8.72777698721907	-3.27856300596744
H	0.03445199568702	7.58455500143747	-3.20734099977881
H	0.03443298695018	2.14545401614461	-3.23346500737004
H	0.03441200367748	-3.29794397598100	-3.26543400214474
H	-3.81718099708196	2.14017399797370	-3.23817001615442
H	-3.81719500135623	-3.29399601730821	-3.25725198369993
H	3.88603898093489	2.14017302034448	-3.24351096750928
H	3.88602500334323	-3.29399600775637	-3.26259201695815
H	-5.11337400572584	3.99839900640055	-1.91683199366782
P	-5.74790338158489	-0.96441632426778	-1.89735767741288
P	1.95386173958685	4.46428181619252	-1.88506765025889
P	1.97957562948438	-0.95950271052070	-1.90747568489696
P	1.96680619046230	-6.40933334616253	-1.93704414873421
H	1.35154400376519	9.45881400004467	-1.88431099849435
H	-7.02727600388658	1.21824096975726	0.00915001484051
H	7.10063298860721	1.21824000019553	-0.00064700405479
P	0.03677929176549	-9.19218153454556	-0.02633486830779
P	0.03673827461330	7.22333164130441	0.01522202459410
P	0.03287115121802	1.75252781120499	0.00257557633229
P	0.03661488445975	-3.65611596243204	-0.02569984309794
H	-3.18266698538389	6.67007199043152	0.04318399761249
P	-3.80486678070652	1.76709643206353	0.01351814352553
P	-3.89241868526629	-3.66058675685820	0.02340695745765
H	3.25607699075949	6.67007199927432	0.03871999750000

P	3.86333395172564	1.77480617387582	-0.00439029340443
P	3.93428535778336	-3.69566676765268	-0.00769506484376
H	-5.10938396846403	4.19249399026272	1.97109298662814
P	-5.83116296415813	-0.77643292832569	2.19880852841319
P	1.92710329661472	4.62247698271216	2.21347454545410
P	2.03763961497309	-0.82706373758152	2.13507344247340
P	2.00956993293310	-6.25938334110054	2.11224345523770
H	1.34349999354455	9.64520400181316	2.00665300229125
O	-4.00293224638200	-3.61265025718447	3.41143847635407
H	-1.90284527503067	-0.21543119522380	2.97929575885738
H	-4.07299916302432	-3.16778308421355	4.27006118557130
C	1.43765630416602	-4.37851352808294	5.40732619262943
C	1.36132355679744	-3.65528733434785	4.22689899020576
C	-0.96449914146402	-3.80050588545478	4.20139773943994
C	-0.96217488808661	-4.52747103474325	5.38599803502850
C	0.25434995253014	-4.82231431073175	6.00082326939128
H	0.28221978614816	-5.38956079282643	6.92450623391058
H	-1.90400656871976	-4.86109938388749	5.80516195006208
H	-1.89766216831176	-3.56774368400340	3.69879409541740
H	2.25074997181513	-3.28213115406393	3.73541531299174
H	2.40537859221887	-4.59466406747031	5.84296867509048
N	0.18164453923164	-3.36526056366473	3.63490243256857

Adsorbed Py+OH⁻

Energy=-8590.09409240365

H	-1.89126797751110	5.22936299935980	-3.08239699617957
H	-1.89129301127233	-0.21736697962785	-3.11949100957423
H	-1.89131802099443	-5.66540501116206	-3.15456000559782
H	5.81192802102604	-0.21877900699642	-3.12273900246380
H	-1.10798497910691	-10.03481499360054	-0.05366498330267
Ga	-1.86516457596853	5.85908508656489	0.09430830430413
Ga	-1.91545353808158	0.35271733725349	0.15121799598252
Ga	-1.93780990801392	-4.96815035566855	0.11693632952291
Ga	5.79014333228390	0.44089705038794	0.13661111205871
H	5.03736899801071	-4.59106700208635	-0.02090001548595
H	-5.74290197446555	-0.21877798680710	-3.11472599296660
H	1.96034202237590	5.22936299728639	-3.08506700383837
H	1.96031700539783	-0.21736798189194	-3.12215999991783
H	1.96029200254595	-5.66540400922570	-3.15723099413576
H	-6.89107803542386	-1.81629000698961	-1.95500299707721
H	6.96171098345034	-1.81629198344636	-1.96460700393979
Ga	0.02865428616892	3.08191555041790	-2.00254073266284
Ga	0.01983564431299	-2.34347425715938	-2.02593551893658
Ga	0.02182971080131	-7.83047747325238	-2.04421854780782
Ga	0.03528607181159	8.58417119147055	-1.99895597988253
Ga	-3.84219017627536	3.08773678429957	-2.00063595178665
Ga	-3.83866709193289	-2.38957008431914	-2.00387944292738
H	-3.03830900372510	-7.26237000571524	-1.99458000829587
Ga	3.90813915264295	3.10147981926970	-2.01846849353258

Ga	3.89525858817389	-2.36617651034898	-2.03675099833995
H	3.10889199494723	-7.26237199376023	-1.99884199958729
Ga	-5.72348211650147	0.40711668030941	0.16891971202221
H	-4.96404286951626	-4.59106689795177	-0.01396703449914
H	1.18125897818107	-10.03481398928922	-0.05525200059604
Ga	1.93621214810644	5.86160591795594	0.09350781814537
Ga	1.94319601820740	0.41343286181806	0.09867185538247
Ga	1.94914704271244	-5.00742527350694	0.09590981791358
H	-6.91692906108794	-1.58514999620422	1.75643501172799
H	6.99270999417815	-1.58515199134405	1.74679199813824
Ga	0.03028365574094	3.39726168337687	1.63277688656382
Ga	0.02293121042100	-2.14369362326990	1.87429926660004
Ga	0.02360194093005	-7.47089602073436	1.65209682950325
Ga	0.03769830802357	8.93075821084809	1.55678193472177
Ga	-3.75829100569369	3.46078244215346	1.59664149088590
Ga	-3.93200054191272	-2.24824128371927	2.02711379534281
H	-3.06396402573169	-7.03126003031373	1.71723300063842
Ga	3.83034884062166	3.47088309779141	1.59376677524297
Ga	3.97776901367944	-2.00195301708470	1.65664763274135
H	3.13969401368107	-7.03126100259992	1.71293200224565
P	-1.88572355157480	4.45926667599831	-1.88492413587217
P	-1.91655206708071	-0.96262412110588	-1.90275608465774
P	-1.90677831790617	-6.39139160388253	-1.91971551679675
H	-1.28080399428295	9.45881399721986	-1.88248500009861
H	5.18406497377852	3.99839997584094	-1.92397101704236
P	5.81385046373831	-0.96746900726813	-1.90473942004019
P	-1.85518590032947	4.61704588003159	2.21462156260165
P	-1.94812399866594	-0.89705413881189	2.15207682197211
P	-1.94087532359078	-6.25423062501592	2.12495110183979
H	-1.26736699177123	9.64520400402859	2.00846299919457
H	5.18546298841459	4.19249399806784	1.96395598859207
P	5.89833899161142	-0.79492024769818	2.19751297311379
H	0.03440201086582	-8.72777699170323	-3.27856300368180
H	0.03445199780689	7.58455500513765	-3.20734099514946
H	0.03443298593947	2.14545399089201	-3.23346500725763
H	0.03441199243231	-3.29794400905417	-3.26543397127053
H	-3.81718099353337	2.14017397527599	-3.23817003024552
H	-3.81719500913863	-3.29399602835740	-3.25725197310593
H	3.88603900843585	2.14017303270330	-3.24351096078886
H	3.88602501068818	-3.29399600750633	-3.26259199557517
H	-5.11337401091111	3.99839901246770	-1.91683198230281
P	-5.74258914564666	-0.96736046527875	-1.89675922749706
P	1.94827310608512	4.45936618082881	-1.88664008308513
P	1.96817859837514	-0.96097627067025	-1.90757449039545
P	1.96730265984978	-6.40555884427423	-1.93300920469926
H	1.35154399565690	9.45881399626581	-1.88431100031111
H	-7.02727599112684	1.21824096803172	0.00915000125649
H	7.10063296220940	1.21823997308030	-0.00064699918505
P	0.03646493176407	-9.19041902234169	-0.02819457371834

P	0.03545904937598	7.21890078253356	0.01596414264967
P	0.00705004104566	1.73785700603336	-0.00217157702828
P	0.02768218317313	-3.64256309664848	-0.01282220647854
H	-3.18266701215911	6.67007201082737	0.04318399964622
P	-3.79457276727153	1.75664063359691	0.00592714107162
P	-3.89631350431684	-3.64802250736305	0.03518806980898
H	3.25607698219711	6.67007199092775	0.03872000269940
P	3.85596892674807	1.76931167671202	-0.00632082054565
P	3.93092927871227	-3.69876235088980	-0.00927344065209
H	-5.10938394014809	4.19249398084005	1.97109297941404
P	-5.81214275985618	-0.79035169342063	2.18567932528283
P	1.92281294397523	4.61292986623468	2.21049884968730
P	2.00136444044987	-0.84936547317152	2.11839145323823
P	2.00849582061817	-6.26149749610279	2.11354585099262
H	1.34349999194130	9.64520400177411	2.00665300200671
O	-4.01655198394324	-3.59150814921302	3.37265039367878
H	-4.02418038577718	-3.15912554551414	4.24040996505122
C	1.47190373168532	-4.37762928366081	5.35535467731029
C	1.35321394230135	-3.64909735676839	4.17968524007006
C	-0.96745237849453	-3.80505850519723	4.22496443976858
C	-0.92592650398692	-4.53944954668714	5.40478637974287
C	0.31018456878820	-4.83028089107324	5.98245303917716
H	0.36947906399498	-5.40049255000555	6.90308124764221
H	-1.85188097284216	-4.88400435755844	5.85021152162012
H	-1.91395579119196	-3.57641672265274	3.74504066054859
H	2.22475302729507	-3.27264162308121	3.65969250079976
H	2.45393397533451	-4.59345856246932	5.75854956122876
N	0.15766533832115	-3.35978275374832	3.62656366056447

Adsorption energy study on implicitly solvated, bare, neutral cluster

1) PyH⁺

Energy=-8514.56251368427

H	5.77741511096763	18.48719925822658	2.80454887708882
H	5.77741500262398	13.04046336050259	2.76833020901755
H	5.77741486405679	7.59242004301967	2.73413667989093
H	13.48063506707076	13.03905259749224	2.77042344987457
H	6.55859731684859	3.22350849187940	5.83627543257339
Ga	5.80433867095601	19.13240776467649	5.97465055979508
Ga	5.77214463486739	13.68955243482749	5.97717399846166
Ga	5.74778895719988	8.22050510508786	5.97306875484959
Ga	13.46631528567399	13.68951603717233	6.03366246592887
H	12.70392628544318	8.66726174974948	5.87242507014423
H	1.92580494162712	13.03905176228826	2.77042467173369
H	9.62902517546317	18.48719936687553	2.80454878225661
H	9.62902502921544	13.04046305452665	2.76833075555163
H	9.62902495558927	7.59242096519562	2.73413538819388
H	0.77682477209907	11.44172609146863	3.92960751400115
H	14.62961389332425	11.44172601409958	3.92960800080100
Ga	7.70319004817913	16.36386413933408	3.86315848177274

Ga	7.70321264010273	10.93719530207173	3.82370284854864
Ga	7.70296376711385	5.40786785047635	3.85319999829907
Ga	7.70315608735440	21.84829391235094	3.88138524367688
Ga	3.82697685456466	16.36456548164626	3.86374639581105
Ga	3.82379207373824	10.89436166649316	3.84628986467350
H	4.62962034885405	5.99564061744326	3.89357730672040
Ga	11.57948786869681	16.36453276799703	3.86370608041213
Ga	11.58236699999375	10.89416328707198	3.84652883319444
H	10.77682042565310	5.99563929329174	3.89357707415870
Ga	1.94038893011396	13.68987755015055	6.03386746199727
H	2.70251342866907	8.66726132402324	5.87242543311009
H	8.84784140300333	3.22350891518532	5.83627574455136
Ga	9.60232207820373	19.13253827055251	5.97377178532000
Ga	9.63420777404160	13.69001799593376	5.97745509778151
Ga	9.65889707660580	8.22034076709802	5.97288809228225
H	0.74840070927059	11.67346251898564	7.64098898151941
H	14.65803967742047	11.67346264661680	7.64098962194120
Ga	7.70323579021029	16.70582068954945	7.50950020677469
Ga	7.70386691543535	11.19015752620530	7.45520330357112
Ga	7.70322136593314	5.77800514374454	7.56962554911032
Ga	7.70326893519692	22.19324212319055	7.44909355506119
Ga	3.91416346674240	16.74915138742837	7.48613894429914
Ga	3.74414125084845	11.22018438966625	7.56907345642328
H	4.60139087239931	6.22734725470077	7.60533347783938
Ga	11.49257736703070	16.74941298777342	7.48485693321602
Ga	11.66072043942020	11.22156968796436	7.56919311174470
H	10.80504971078193	6.22734636498962	7.60533301749005
P	5.78428997416074	17.72258090896724	4.00349477848530
P	5.75813837752509	12.30224580628750	3.98451117909295
P	5.77064059653295	6.84481232632878	3.95202477855572
H	6.38704571578321	22.71684346064575	4.00420318969224
H	12.85194068304549	17.25642361031651	3.96807759170497
P	13.48690684895568	12.29496650735499	3.98896439903869
P	5.81591338393038	17.89201573315996	8.11162192392593
P	5.75867767631865	12.36582621019340	8.00538968082264
P	5.72581284351153	7.01018263896693	8.01046404056149
H	6.39778572646921	22.90385779295503	7.89512879563188
H	12.85064302666230	17.45114207127183	7.85597213374337
P	13.56186620587770	12.46267855220375	8.09627550551594
H	7.70321977815320	4.53002824977379	2.61196073681647
H	7.70321988617211	20.84237172560648	2.68056184170786
H	7.70322003865891	15.40326654964936	2.65531109743780
H	7.70321992703984	9.95986313966057	2.62421713755141
H	3.85161006275657	15.39798395132483	2.64793620072133
H	3.85160994978518	9.96381132661188	2.62972783176336
H	11.55483003226288	15.39798433441760	2.64793736002642
H	11.55482990613306	9.96381193757251	2.62972866915694
H	2.55450145647497	17.25642180325547	3.96807764513576
P	1.91940648096172	12.29516500800643	3.98905508811659

P	9.62213703037430	17.72247474745281	4.00329706709350
P	9.64820877969342	12.30237167291793	3.98462428898526
P	9.63571968196324	6.84458115178960	3.95183585396484
H	9.01939443418370	22.71684275766840	4.00420263595755
H	0.63926638178306	14.47657187452167	5.89317720709734
H	14.76717413541794	14.47657319635311	5.89317634452496
P	7.70320584575642	4.06725059968897	5.87364171336206
P	7.70325792039433	20.48357197082823	5.90352939546967
P	7.70304290447028	15.02676216086073	5.89100042276058
P	7.70349392982111	9.54545758558343	5.79765853088168
H	4.48384938826773	19.92840913263922	5.92900068740444
P	3.87111351773580	15.03505061689479	5.89748389503793
P	3.80259280370336	9.56339074265137	5.87368773142677
H	10.92259225472041	19.92841039287251	5.92900144095670
P	11.53557342077577	15.03487886791604	5.89710315374532
P	11.60383014464884	9.56353980075800	5.87400366118281
H	2.55579667602680	17.45114108058593	7.85597167170901
P	1.84435499938608	12.46266295459475	8.09660015857269
P	9.59099005971871	17.89281948789570	8.10921724402959
P	9.64695841463790	12.36867078277465	8.00730777881558
P	9.68063597888898	7.01015747726941	8.01043923572076
H	9.00865316180476	22.90385833388493	7.89512910320940
C	6.46024630505443	16.19555126863847	11.22242735123838
C	6.48054187744332	15.04392545473378	10.45468687743868
C	8.85770161954773	15.05462261079254	10.43094072971165
C	8.88230658156245	16.20626646559054	11.19886360982740
C	7.67265512991102	16.77939337008302	11.60285050458530
H	7.67468795081791	17.67982856061644	12.20541553922512
H	9.83209418259281	16.64491313500744	11.47276021981664
H	9.73278746086479	14.52672990766978	10.07626620163492
H	5.60350304157080	14.50844134203433	10.11692304240216
H	5.51205644764082	16.62568302762480	11.51497514673280
N	7.66797273003546	14.51309267164521	10.09208140703513
H	7.66429309062308	13.64578977428299	9.55032362532599

2) CO₂

Energy=-8454.4435002588

H	5.77741500254181	18.48719900378358	2.80454900641991
H	5.77741500522212	13.04046302558078	2.76833001564224
H	5.77741498553809	7.59241998449399	2.73413700629827
H	13.48063497194713	13.03905302501812	2.77042299708538
H	6.55859701261528	3.22350899327587	5.83627499957800
Ga	5.80429052991151	19.12533565467982	5.98835923045543
Ga	5.77277059890100	13.69331897187798	5.98809242584693
Ga	5.75261085044070	8.22714189519399	5.97509753412422
Ga	13.46311796050965	13.69260690164183	6.03650193670416
H	12.70392599005989	8.66726200349887	5.87242499300850
H	1.92580502337588	13.03905203507112	2.77042497620607
H	9.62902499456082	18.48719900309931	2.80454900433622

H	9.62902499356015	13.04046301343185	2.76833100069123
H	9.62902501536471	7.59242098452259	2.73413500492266
H	0.77682497103175	11.44172597438063	3.92960801943855
H	14.62961401854539	11.44172597947849	3.92960800561643
Ga	7.70309868902855	16.35818835711098	3.87054036690643
Ga	7.70329413647899	10.93739969376119	3.82731647080838
Ga	7.70309816418318	5.40921793268337	3.85277352535195
Ga	7.70329427003679	21.84511529562096	3.88520171062371
Ga	3.82962160968451	16.36336096928562	3.86788813371874
Ga	3.82844905531841	10.89624692160701	3.84629572039431
H	4.62962001722882	5.99564101736859	3.89357699659249
Ga	11.57693888662282	16.36349959571471	3.86774871844918
Ga	11.57857696979425	10.89626617838122	3.84619729760798
H	10.77682098272319	5.99563901521694	3.89357699765964
Ga	1.94320415772060	13.69249878740893	6.03669843652405
H	2.70251301198103	8.66726101442130	5.87242499918594
H	8.84784098621108	3.22350900902664	5.83627600044862
Ga	9.60217327599910	19.12520147930611	5.98837456413594
Ga	9.63361441206987	13.69315368607543	5.98664015524973
Ga	9.65391890574905	8.22708440748533	5.97510619510339
H	0.74840102342786	11.67346300313427	7.64098900448832
H	14.65803998041726	11.67346300197519	7.64099000418750
Ga	7.70385086267373	16.66318903007413	7.55063969294017
Ga	7.70348376296953	11.21269353140764	7.47455579402634
Ga	7.70318125194289	5.77806821265118	7.56783124848401
Ga	7.70324763629378	22.19312169168570	7.44506937578641
Ga	3.91325145591293	16.73965065179760	7.49979014343828
Ga	3.74865820879594	11.21796384838673	7.55631173845093
H	4.60139099413732	6.22734699433148	7.60533300061330
Ga	11.49354445474879	16.73888536087765	7.49976004915192
Ga	11.65691272857553	11.21890464816365	7.55618224948306
H	10.80505000333858	6.22734599811599	7.60533300074544
P	5.78542667909748	17.72347030508565	4.00564805813786
P	5.75899271887199	12.30563714646554	3.98721945606374
P	5.77069840451830	6.84595134629506	3.95324355959886
H	6.38704596322569	22.71684298279465	4.00420299623004
H	12.85194099984350	17.25642398998029	3.96807799628932
P	13.48690837411009	12.29525949935023	3.98962723626505
P	5.81642873556187	17.88490562328401	8.11100925601814
P	5.74306678525075	12.36952022331742	8.01324202425602
P	5.72617750765972	7.00940232945544	8.00902982441326
H	6.39778625061343	22.90385802003584	7.89512894335819
H	12.85064297180204	17.45114198366362	7.85597199076403
P	13.55880673526911	12.45733081217092	8.09402166562966
H	7.70321999769424	4.53002799521975	2.61196098439168
H	7.70322008270548	20.84237208774928	2.68056209929471
H	7.70321999909487	15.40326600130176	2.65531101318004
H	7.70321999724224	9.95986298820405	2.62421701507320
H	3.85160999227282	15.39798399943913	2.64793600940866

H	3.85161000299712	9.96381094977118	2.62972797564163
H	11.55482999818820	15.39798400722504	2.64793701285775
H	11.55483000721941	9.96381196960670	2.62972899591161
H	2.55450101032043	17.25642199068020	3.96807799860029
P	1.91965488619187	12.29511201102381	3.98957983212605
P	9.62098436164989	17.72333454186117	4.00560692709700
P	9.64770570854678	12.30531370259905	3.98678635787162
P	9.63572247040483	6.84578861246533	3.95311119885614
H	9.01939392352243	22.71684294615303	4.00420297374242
H	0.63926594350117	14.47657202520075	5.89317700112158
H	14.76717404279658	14.47657302401589	5.89317600041370
P	7.70319997788193	4.06717952837313	5.87264529446596
P	7.70325005928575	20.48082334448129	5.90383250904738
P	7.70326457246298	15.02611362442684	5.88847276156916
P	7.70328766652139	9.55907884094735	5.81037081991927
H	4.48384898838594	19.92840899938595	5.92900100319856
P	3.87004672139148	15.03660815194885	5.89662983707204
P	3.80217274976712	9.56024688406765	5.86883391800180
H	10.92259302634475	19.92841101992086	5.92900100089130
P	11.53631766526647	15.03654355284833	5.89607330035963
P	11.60422990753530	9.56033820907327	5.86894082109761
H	2.55579703632422	17.45114098320903	7.85597198912776
P	1.84747025907158	12.45738621070442	8.09420144939691
P	9.59089131620388	17.88464444606320	8.11190881694122
P	9.66274703809554	12.37190283833758	8.01242844603843
P	9.68018056440381	7.00930142179979	8.00908897778509
H	9.00865276448382	22.90385792485651	7.89512896295808
O	7.67243204156932	14.86905747360547	9.69922505418946
O	7.73420368653502	12.87843426731488	10.92567071914149
C	7.70480389260064	13.86358189054716	10.29936030645140

3) HCOOH

Same structure as the one reported in “pK_a calculations” section

4) H₂O

Same structure as the one reported in “pK_a calculations” section

5) o-DHP

Same structure as the one reported in “pK_a calculations” section

6) Py

Energy=-8514.12500511984

H	5.77741511628447	18.48719923090386	2.80454890783753
H	5.77741498981278	13.04046333145948	2.76833019005996
H	5.77741488149736	7.59242005745562	2.73413667268404
H	13.48063510035502	13.03905257906895	2.77042345889198
H	6.55859731704283	3.22350849558597	5.83627543153594
Ga	5.80479050811889	19.11172104543578	5.99727577462022
Ga	5.79785891553593	13.70491466303460	5.99795611591768

Ga	5.75383421193488	8.22943714054909	5.97345543914500
Ga	13.45816139692369	13.69883594768403	6.04006052918947
H	12.70392629527662	8.66726175036537	5.87242507408977
H	1.92580491229806	13.03905173306291	2.77042469215633
H	9.62902518475769	18.48719934693155	2.80454878458662
H	9.62902503361189	13.04046302063252	2.76833075202718
H	9.62902494132580	7.59242098211474	2.73413538136169
H	0.77682479701825	11.44172611334661	3.92960749017222
H	14.62961387246201	11.44172603310291	3.92960798836867
Ga	7.70347454614950	16.34464405570244	3.89246851412475
Ga	7.70307766012580	10.94125698531683	3.82614889086719
Ga	7.70296561275489	5.41071028535596	3.85159007384901
Ga	7.70319752662818	21.83943464358999	3.89276129428078
Ga	3.83469492036157	16.36397265714145	3.87211391464545
Ga	3.83244192800126	10.90202593918655	3.84398310506542
H	4.62962032638055	5.99564059677965	3.89357730855754
Ga	11.57182050503793	16.36391780885632	3.87209110771101
Ga	11.57377498910267	10.90171647287719	3.84421270618471
H	10.77682044902661	5.99563927627740	3.89357707546958
Ga	1.94867236957118	13.69942752418744	6.04046453547761
H	2.70251341401608	8.66726130640638	5.87242542887151
H	8.84784140361721	3.22350891079094	5.83627574223403
Ga	9.60170047155824	19.11153119346404	5.99786616786369
Ga	9.60873524395537	13.70523883822685	5.99790170856149
Ga	9.65258604312311	8.22943525643120	5.97347277546410
H	0.74840068755809	11.67346251020873	7.64098897580574
H	14.65803970133848	11.67346263776446	7.64098961665743
Ga	7.70331709738122	16.56489120994008	7.77515722120221
Ga	7.70324377828664	11.21627038269708	7.47349541895902
Ga	7.70312170702628	5.78037738938904	7.56820681063998
Ga	7.70322930642842	22.18681103991387	7.44459472923630
Ga	3.92101142854796	16.75520273794838	7.49752798649134
Ga	3.76041417160066	11.22274446887924	7.54171935816538
H	4.60139088203822	6.22734725985188	7.60533347845862
Ga	11.48585568714329	16.75438692755269	7.49720513383129
Ga	11.64579867288939	11.22335836445624	7.54182861141773
H	10.80504970309584	6.22734636686523	7.60533301797742
P	5.78931751100521	17.72252855267596	4.00536295424390
P	5.76127012125978	12.31252870208790	3.99145571164378
P	5.77091831598230	6.84574953497103	3.95302181858630
H	6.38704566722708	22.71684349048513	4.00420320460745
H	12.85194064881153	17.25642360234891	3.96807759065771
P	13.48632261637929	12.29649479398533	3.99085851259892
P	5.81196114626980	17.90625987999608	8.10237087429325
P	5.74490176372177	12.36719682434194	8.01900162274984
P	5.72577591039895	7.01094367655555	8.00915164763516
H	6.39778561487996	22.90385777507683	7.89512882974355
H	12.85064306781604	17.45114209183900	7.85597216197027
P	13.55302681214221	12.45266386688021	8.09063389163287

H	7.70321977887786	4.53002825265203	2.61196075316137
H	7.70321985148710	20.84237161342600	2.68056174177341
H	7.70322003702147	15.40326648442178	2.65531101316733
H	7.70321992968329	9.95986315624384	2.62421712413374
H	3.85161006250456	15.39798397135286	2.64793619894454
H	3.85160994822397	9.96381136417725	2.62972785470662
H	11.55483004117588	15.39798434368433	2.64793736122903
H	11.55482990070448	9.96381196097068	2.62972866984035
H	2.55450146989017	17.25642179506978	3.96807764185063
P	1.91996135150589	12.29675469166200	3.99100598867535
P	9.61733337614039	17.72259932332950	4.00549838904250
P	9.64503013731703	12.31249056661593	3.99143143008144
P	9.63544357502338	6.84560467907362	3.95288568492034
H	9.01939453747798	22.71684281658102	4.00420266419537
H	0.63926645508374	14.47657184893127	5.89317720244623
H	14.76717407069932	14.47657316820655	5.89317634440572
P	7.70320736135020	4.06781086622825	5.87241650977065
P	7.70337127358609	20.47537975685913	5.90520619556851
P	7.70319984899396	15.07068924386622	5.92976988998853
P	7.70328965246893	9.55889056191509	5.80774430743698
H	4.48384919210094	19.92840920548535	5.92900070688857
P	3.87868901264299	15.03639227639420	5.90522182141326
P	3.80288278653585	9.55856985218514	5.86323685056982
H	10.92259242173363	19.92841045063856	5.92900145969116
P	11.52818865119740	15.03601096093292	5.90481442428081
P	11.60359699424674	9.55856230342257	5.86341772614754
H	2.55579664997941	17.45114110045140	7.85597168397178
P	1.85354034609484	12.45247528168533	8.09069053617231
P	9.59501851941737	17.90538990303211	8.10271730554076
P	9.66128313965962	12.36799665268436	8.01950647039855
P	9.68056254873443	7.01083839448309	8.00909919117097
H	9.00865326308198	22.90385836525497	7.89512911934330
C	8.90573298568214	14.17406664533829	11.25168442336742
C	8.86356798572188	14.94189498925789	10.09482243050066
C	6.54256972128961	14.94350738488331	10.09572942518726
C	6.50018896618411	14.17598920521099	11.25269396851805
C	7.70293010001131	13.78604708338258	11.84357223204942
H	7.70293644720119	13.18785699889688	12.74827174390624
H	5.54440237410025	13.88485786558156	11.67144235136431
H	5.63838972578715	15.27789593303738	9.60210591022929
H	9.76788245047310	15.27503842810848	9.60057074971020
H	9.86143279778370	13.88143427181701	11.66957282781321
N	7.70316840254910	15.33101873362505	9.53155698495415

7) HCOO⁻

Same structure as the one reported in “pK_a calculations” section

8) OH⁻

Same structure as the one reported in “pK_a calculations” section

9) H₂O + H⁺

Same structure as the one reported in “Co-adsorption effect” section for H₂O co-adsorption study.

Adsorption energy study on explicitly solvated, neutral cluster

1) PyH⁺

PyH⁺ on explicitly solvated surface

Energy=-8973.13837389644

H	5.77741506879307	18.48719925039952	2.80454894580410
H	5.77741497730482	13.04046344933738	2.76833019934197
H	5.77741493358043	7.59242008619690	2.73413665719432
H	13.48063516067404	13.03905256497290	2.77042346980067
H	6.55859733777635	3.22350848684228	5.83627542994475
Ga	5.81149754518478	19.14816949207951	5.87795193625997
Ga	5.72949499549310	13.81591470292242	5.78397792553823
Ga	5.74305492383694	8.26117466346185	5.99199319843281
Ga	13.44705793884459	13.68834565062172	6.03759497510686
H	12.70392633126933	8.66726170687560	5.87242509520135
H	1.92580496247658	13.03905188603964	2.77042450486171
H	9.62902517291930	18.48719931019962	2.80454877356606
H	9.62902503582115	13.04046313314770	2.76833076594882
H	9.62902482396948	7.59242107051452	2.73413535396652
H	0.77682473114105	11.44172597242473	3.92960758025003
H	14.62961380450047	11.44172609110145	3.92960797746852
Ga	7.73690380708360	16.38066439768868	3.84808507389514
Ga	7.71258637753764	10.92497860794397	3.84863181984392
Ga	7.69237441561045	5.41803888358430	3.84700059348559
Ga	7.70445186224937	21.83072408056504	3.90962089900986
Ga	3.80741082008392	16.35952285633045	3.87406943551374
Ga	3.80923555934083	10.87691973953549	3.86936084057675
H	4.62962026518412	5.99564055201365	3.89357731131518
Ga	11.58774772036103	16.34609770816120	3.88113453153691
Ga	11.59395980369467	10.88574007865654	3.85591489402430
H	10.77682057856032	5.99563916365596	3.89357708602995
Ga	1.95650770825613	13.66880201354757	6.02750876971698
H	2.70251338995044	8.66726129712650	5.87242545789749
H	8.84784137203868	3.22350891293204	5.83627573327067
Ga	9.60647344840669	19.11476828834621	5.98157004574114
Ga	9.65038961748387	13.62451351103119	5.97851991186364
Ga	9.65391014855871	8.26028101508807	5.94790051264737
H	0.74840063902536	11.67346246646193	7.64098896845936
H	14.65803971723741	11.67346264978748	7.64098960963349
Ga	7.84061969786918	16.61253688294302	7.51024171077948
Ga	7.71820195829605	11.09889364083449	7.74800051748520
Ga	7.68825972141145	5.77654769306324	7.55345406739701
Ga	7.70958364824388	22.05692993183234	7.65772238562214
Ga	3.72529443829784	16.37981946497266	7.89985400883429
Ga	3.68574027496850	10.99375875377880	7.85139162492332
H	4.60139091001443	6.22734726992517	7.60533347710513

Ga	11.54095417338808	16.58607351298877	7.67728883199371
Ga	11.62256809621137	11.09866849225342	7.74648716079660
H	10.80504967335479	6.22734637227683	7.60533301810194
P	5.78386843933994	17.69721717759931	3.98032361137291
P	5.75604857204196	12.28688193743396	3.95791544442472
P	5.76536599246409	6.85903990976801	3.96245852724186
H	6.38704564715144	22.71684347781411	4.00420320524133
H	12.85194061464026	17.25642354858456	3.96807755509512
P	13.48835308924150	12.29688447475475	3.98996202735252
P	5.78193121807432	17.64309758460444	7.81766760455670
P	5.69139450583534	12.34056557880602	7.60954690676783
P	5.72969290732267	7.00534565947244	8.01193161253289
H	6.39778601866306	22.90385783177101	7.89512874341957
H	12.85064293231670	17.45114196861552	7.85597214548351
P	13.53473487296988	12.43806132885427	8.07432254065390
H	7.70321979528243	4.53002828856321	2.61196080154458
H	7.70322001464131	20.84237179537921	2.68056193408523
H	7.70322004045286	15.40326648595714	2.65531100467675
H	7.70321993479845	9.95986301691576	2.62421710109265
H	3.85161011057388	15.39798387484583	2.64793613607178
H	3.85160995512363	9.96381132345850	2.62972786200509
H	11.55483005100672	15.39798442314566	2.64793744541034
H	11.55482990476229	9.96381193657280	2.62972869672582
H	2.55450141035563	17.25642186909811	3.96807766564422
P	1.91889205702244	12.29254808201299	3.98650420089218
P	9.64404159793341	17.72472507870397	4.00142412716511
P	9.65529579197915	12.28385853456607	3.97387798652702
P	9.63213545158771	6.84705269892589	3.95151399730904
H	9.01939432081479	22.71684266269095	4.00420261243563
H	0.63926650425582	14.47657189040495	5.89317727168549
H	14.76717409482772	14.47657316836593	5.89317633197647
P	7.70481944143871	4.06729743885692	5.86459608482976
P	7.71327157939001	20.48659898720894	5.91625268888390
P	7.74166613776553	15.01205171595117	5.84618292504291
P	7.69738638973302	9.61875110636737	5.87000932085205
H	4.48384917985078	19.92840911907508	5.92900073045001
P	3.82413759504700	15.10156454312822	5.89019292775269
P	3.78355178961227	9.58841428150657	5.90811520597141
H	10.92259275183942	19.92841070565660	5.92900142224179
P	11.51797397032762	15.03985007459582	5.89122684015656
P	11.61386962088073	9.58427765052500	5.88423989388804
H	2.55579658365211	17.45114113235971	7.85597169953047
P	1.85708018980688	12.45571879557791	8.08023968862501
P	9.62486001337295	17.88454941368818	8.13027946859699
P	9.66082280018125	12.40160495151163	8.04153251913955
P	9.67524160365943	7.01545856761410	7.97723269344806
H	9.00865287196511	22.90385820593333	7.89512904630468
O	4.43855657279383	9.97735930383340	9.32223754642229
O	6.94522478059077	10.05541574215831	9.34957656134933

H	5.60515817687023	13.23844452975968	8.69118734105097
H	4.04040698387823	10.18585270093736	10.18136076990674
H	5.86996120234569	9.99425832600699	9.36601877184428
H	7.29607005909844	9.18207651918991	9.58558201004901
H	5.96738490395731	18.50007307655930	8.92347086575759
O	3.86509338423058	15.23905056386919	9.40897836534351
H	3.27426456254238	14.47448586895226	9.31844927058967
O	7.93583528369317	20.67039331901416	9.30897470658902
H	8.50805817772732	19.90315226298384	9.08273937629717
H	7.10454633607502	20.30071967046771	9.64576191897621
O	11.59884030445385	15.06068608052439	9.25049114436706
H	10.91386268444368	14.37416521369699	9.09489845750368
H	12.44533295088890	14.57096418501553	9.25349574876961
O	11.32481268631196	9.73573172062491	9.35024402656660
H	10.83824794405103	8.91123710710846	9.13433505894342
H	12.12276956644455	9.45701752396331	9.83020525883534
C	7.55624691569157	15.84572348578550	10.69797964395948
C	6.69137634371491	14.77388413071507	10.55539870410372
C	8.42675985906356	13.26713843426628	11.18729752881993
C	9.31931191156824	14.31571651771922	11.34216166709290
C	8.88123599209280	15.61749292808731	11.09449485014886
H	9.56379191583463	16.45187918646215	11.20375088100766
H	10.33663700735056	14.10740756687687	11.64494509259547
H	8.67799504918198	12.23071235329598	11.36115998766033
H	5.64746598339747	14.86840892948229	10.24330462769748
H	7.18867874202347	16.84727226955632	10.51425684200539
N	7.15745737700848	13.52886618463607	10.81712653661115
H	6.52404400537956	12.74256716198709	10.70996378764112

Explicitly solvated surface without PyH⁺

Energy=-8724.51667517733

H	-1.93139900988870	5.16831499666156	-3.18721299278646
H	-1.92298199968140	-0.27851302939548	-3.20954199360141
H	-1.91455697216833	-5.72664397563700	-3.22984401687490
H	5.78024600374158	-0.26786100156534	-3.23053100272550
H	-1.11723898004941	-10.08642197758415	-0.11890500384862
Ga	-1.89238745946324	5.82812639835286	-0.10649232868189
Ga	-1.95952524884770	0.49345733410847	-0.15661628986621
Ga	-1.94014041833871	-5.04722142915910	0.01959618767705
Ga	5.75432087706753	0.39003032519154	0.03893113991763
H	5.01967798250675	-4.63295699722127	-0.11505499481107
H	-5.77458395811092	-0.28594797342366	-3.19590100850663
H	1.92021100745745	5.17434499775551	-3.19875599132210
H	1.92862800629415	-0.27248401927507	-3.22108500763477
H	1.93705298388981	-5.72061298926208	-3.24138801460982
H	-6.91759004371161	-1.88211603249351	-2.02920198546956
H	6.93519899292833	-1.86043299813723	-2.07071799964536
Ga	0.03233907766688	3.05925690005790	-2.13552304759270
Ga	0.01687228346175	-2.38485906378076	-2.13227252617067

Ga	0.00767793224317	-7.89286773465051	-2.11909301151260
Ga	-0.00650493738199	8.51448248924340	-2.09223747959079
Ga	-3.89324344074954	3.03521211690379	-2.09785784996839
Ga	-3.87991801808681	-2.44066507515719	-2.09573897351155
H	-3.05637702862787	-7.32226302865276	-2.06289098645784
Ga	3.88339977351453	3.03687542196315	-2.11810898396835
Ga	3.89545811851387	-2.41940337664681	-2.13304080752464
H	3.09082301323918	-7.31264201440206	-2.08131398628760
Ga	-5.73071407325928	0.35578382688901	0.06485543774714
H	-4.98173598667907	-4.64861299145506	-0.08508000949833
H	1.17200499052616	-10.08283800139259	-0.12576600133496
Ga	1.90571736528195	5.80814389338173	-0.02050258795106
Ga	1.95483687931703	0.32020219795982	0.00706423900154
Ga	1.97131389981762	-5.04094012059841	-0.03232349698607
H	-6.93525398448186	-1.64096097921808	1.68167299946035
H	6.97438498608511	-1.61918799280627	1.63998799910749
Ga	0.14457134824111	3.30512536244072	1.54020794633362
Ga	0.03061729179482	-2.21838917992417	1.76748456769859
Ga	0.01695932342108	-7.53102645480725	1.58075560163714
Ga	0.00911416887906	8.74935296359079	1.65290201415932
Ga	-3.96281396267370	3.07402816094576	1.93767974630909
Ga	-3.98363004721450	-2.32083612082481	1.90386870166726
H	-3.07384500754819	-7.08113600676672	1.64835800176587
Ga	3.84890619444786	3.28911082534518	1.67569061491140
Ga	3.93877858664698	-2.19269365909225	1.76117121108361
H	3.12981400590987	-7.07142600689989	1.62976499780482
P	-1.92033650659849	4.38081803278433	-2.00869820300744
P	-1.93943253261518	-1.02336852164845	-2.00971522815559
P	-1.92198809624453	-6.45757163006221	-2.00066050912941
H	-1.32479398391660	9.40197299906904	-2.00017100054049
H	5.14853899981331	3.95158000509527	-2.04174799941106
P	5.79207923479578	-1.00707540237343	-2.00854887187200
P	-1.91088065664732	4.34354726199928	1.83768092549658
P	-1.98194690762064	-0.96645336434910	1.68693745443979
P	-1.94050930081486	-6.30693636078996	2.03880515957689
H	-1.30268599402207	9.59892500304475	1.89024500291383
H	5.15858899574441	4.15620999853844	1.84565399526510
P	5.85408685824861	-0.85388369195203	2.07901472901553
H	0.01567499980986	-8.78633200170304	-3.34998199303470
H	-0.00965300442019	7.52618600151300	-3.32297599811020
H	-0.00121500284325	2.08701599798512	-3.33435799959773
H	0.00721200071699	-3.35646597476891	-3.35157100484074
H	-3.85283800884931	2.07568601977080	-3.33017698114796
H	-3.84438701054923	-3.35853298332362	-3.33452799585194
H	3.85038199968623	2.08774499974557	-3.35326099999708
H	3.85883299962113	-3.34647398612082	-3.35761300116375
H	-5.14889998252159	3.93545998596811	-2.01088701362258
P	-5.77589908396683	-1.02869839082064	-1.97669311598925
P	1.93742928650867	4.41372132105564	-1.99956013619127

P	1.95783993755108	-1.02187680232517	-2.00928308590815
P	1.94596147803723	-6.46244152946787	-2.02208471562346
H	1.30755399157302	9.40609299882260	-2.00806000078058
H	-7.05401399619172	1.15752096884818	-0.07295800416279
H	7.07389399982361	1.17963699766801	-0.11530000021377
P	0.02810055638730	-9.24180438561060	-0.10026497140716
P	0.00777729515711	7.17597190098035	-0.08560131218732
P	0.04538218903892	1.70540144575170	-0.13473440354608
P	0.01225660176023	-3.69407030838341	-0.11710421481910
H	-3.21785799024516	6.61546799717127	-0.06255900583858
P	-3.86428192933700	1.78781651972461	-0.07397617991971
P	-3.90178633765884	-3.72324669247349	-0.05270349196686
H	3.22088599026162	6.62554799857427	-0.08185499974311
P	3.82350170319930	1.73534196472257	-0.10536519656838
P	3.92999105662787	-3.71514959926481	-0.09987546386407
H	-5.13625699696029	4.14009500151942	1.87650699793948
P	-5.82337299092520	-0.86070435696182	2.11550098515972
P	1.93672387768492	4.58800395774549	2.12468783071887
P	1.96986923659895	-0.91087078832794	2.06972854162759
P	1.99868280207482	-6.28422333659293	1.99944557679266
H	1.30818198860898	9.60301299661744	1.88242099927894
O	-3.27625905769862	-3.39665102158940	3.35087601806507
O	-0.72567962284777	-3.38282506807576	3.31452872072390
H	-2.00043146951574	-0.10442423240654	2.80277177851428
H	-3.57986501056318	-3.07515006805779	4.21457942938769
H	-1.78246451241326	-3.40766454453001	3.35023052340888
H	-0.41912412088725	-4.29666645447648	3.42682286892885
H	-1.72143815188356	5.22043052582948	2.92562845777947
O	-3.88188067034075	1.97203488995964	3.46363808123126
H	-4.41244306260981	1.17252160923736	3.32267316298945
O	0.23020687055990	7.37509628634980	3.30886243953833
H	0.80701469830975	6.61071883837499	3.08567942973321
H	-0.59749280313438	6.99064203642000	3.63930582228350
O	3.94552683316669	1.82749759783247	3.27391069200774
H	3.22202335383975	1.16946703016326	3.21894695055453
H	4.76508860711259	1.29520276014635	3.26429904024047
O	3.66621576264220	-3.56732116707832	3.37012531785834
H	3.17780650997974	-4.39066407201656	3.15466930034556
H	4.47235069827119	-3.84832991339368	3.83462346726609

2) CO₂

CO₂ on explicitly solvated surface

Energy=-8913.02058830792

H	5.77741510053822	18.48719918949848	2.80454891272998
H	5.77741494324483	13.04046340128594	2.76833019905469
H	5.77741493906051	7.59242009564225	2.73413664814159
H	13.48063509954998	13.03905258369451	2.77042344823410
H	6.55859732258980	3.22350848659543	5.83627542947212
Ga	5.81106512466388	19.14260782431164	5.88413183179135

Ga	5.72838938726694	13.81247332414083	5.80838893614394
Ga	5.74433664825389	8.26373597887957	5.98618437006049
Ga	13.44445084677469	13.69099779620129	6.04315306389322
H	12.70392630238505	8.66726173191670	5.87242508168348
H	1.92580495005439	13.03905184214366	2.77042456377818
H	9.62902517787052	18.48719931539010	2.80454880219224
H	9.62902504282008	13.04046306279315	2.76833079713358
H	9.62902484310603	7.59242104877668	2.73413536328833
H	0.77682475894985	11.44172601759613	3.92960755456670
H	14.62961387197428	11.44172604024551	3.92960798798690
Ga	7.73527508123129	16.37230843517274	3.85736362019932
Ga	7.71012485716865	10.92831951106467	3.84666031446324
Ga	7.69329909849188	5.42060119227579	3.84506837657718
Ga	7.70482423891336	21.82831649318370	3.91291683893313
Ga	3.81027148090603	16.35880749237777	3.87589479174581
Ga	3.81312029440540	10.87942626920196	3.87003302084216
H	4.62962025386357	5.99564053743532	3.89357731140606
Ga	11.58479441579233	16.34474090993816	3.88543787202974
Ga	11.59059245443188	10.88850474072540	3.85600554600772
H	10.77682055233063	5.99563918732410	3.89357708104580
Ga	1.96207609946597	13.67434668005513	6.03033967390186
H	2.70251343471938	8.66726132696851	5.87242543569174
H	8.84784138734197	3.22350891723559	5.83627573935617
Ga	9.60555554164650	19.11161614211204	5.98623553596230
Ga	9.64164700872251	13.62834665005074	5.98905783952732
Ga	9.65113514836932	8.26687363030222	5.94730154763808
H	0.74840065086199	11.67346249228019	7.64098897652915
H	14.65803972727612	11.67346263644014	7.64098961754875
Ga	7.83164462236908	16.59433770187828	7.55211951112708
Ga	7.70735801967139	11.09060275063291	7.75825460024058
Ga	7.69160033217313	5.77224321475352	7.54673943791089
Ga	7.70912254475049	22.05284849737971	7.65732384614696
Ga	3.74079140117710	16.37771482692554	7.90898722775963
Ga	3.69309053499123	10.98557925843498	7.86066143152606
H	4.60139090787886	6.22734726390570	7.60533347767718
Ga	11.53233986529505	16.58951711038462	7.68174141341310
Ga	11.62704242460415	11.09978930598359	7.74962202757597
H	10.80504968112388	6.22734636993382	7.60533301692231
P	5.78486325396757	17.69777156552007	3.98047984569779
P	5.75624058169194	12.29186933973574	3.96371801695894
P	5.76542478544741	6.85861816290757	3.96162662556336
H	6.38704582906369	22.71684344286152	4.00420318814607
H	12.85194062880721	17.25642357502702	3.96807757195331
P	13.48823448516112	12.29769360058732	3.99123955178306
P	5.78274995253074	17.65747234760863	7.81747418090849
P	5.68844198574856	12.34302551602189	7.64252808920177
P	5.73471472822098	6.99884371585249	8.00201521511037
H	6.39778560547394	22.90385772566921	7.89512879676628
H	12.85064303426218	17.45114200836101	7.85597217849738

P	13.53806258762133	12.44007601669212	8.07992214846673
H	7.70321979466810	4.53002828272149	2.61196078936707
H	7.70321986328567	20.84237172607989	2.68056184659150
H	7.70322005424552	15.40326648857834	2.65531097709381
H	7.70321993930889	9.95986305659754	2.62421707133282
H	3.85161005046601	15.39798401871109	2.64793622982260
H	3.85160997656968	9.96381132700508	2.62972788109096
H	11.55483004785102	15.39798437624587	2.64793739469250
H	11.55482989484237	9.96381194884025	2.62972868632258
H	2.55450151310419	17.25642176437875	3.96807762615185
P	1.91921525722186	12.29334355221704	3.98772658775139
P	9.64140688101774	17.72418077341257	4.00199711303177
P	9.65341363297096	12.28717801382762	3.97695629195435
P	9.63300196094355	6.84859923868680	3.95242455250962
H	9.01939436147805	22.71684271163847	4.00420263604407
H	0.63926641446702	14.47657190176160	5.89317725263503
H	14.76717410743607	14.47657319673421	5.89317634626314
P	7.70518324679018	4.06630947075407	5.86082702807751
P	7.71227342832983	20.48675671235867	5.91330647502166
P	7.73610348238857	15.01878622304843	5.85242895494396
P	7.69457547407241	9.62280149173843	5.86566639944642
H	4.48384895551294	19.92840931606462	5.92900071417969
P	3.82607720373684	15.10689756063741	5.88854132300739
P	3.78392501767795	9.58859219283714	5.90846353986173
H	10.92259258125813	19.92841056015211	5.92900143353329
P	11.51523727036905	15.03904121967019	5.89566809253921
P	11.61509493760607	9.58567032191516	5.88515198699115
H	2.55579673655662	17.45114105347456	7.85597165018214
P	1.86068817584873	12.45118874796228	8.07764615707948
P	9.62301187438976	17.89167090366104	8.11871315513267
P	9.65786992636729	12.38463622628980	8.04320088916625
P	9.67383613665991	7.01526122670338	7.97410573200844
H	9.00865328636880	22.90385838943521	7.89512910588568
O	4.41106306316840	9.92660959956613	9.31829775593869
O	6.94542500284527	9.93358947043199	9.29200340115598
H	5.57579173403696	13.22699824883421	8.73614676699655
H	4.08074328129573	10.22341135076151	10.18078038590491
H	5.88196355225924	9.91431521387023	9.32722646762772
H	7.24981883535646	9.01830277699075	9.39937169360918
H	5.95832742854607	18.52837612500382	8.91298517309524
O	3.94694505648176	15.18379186126875	9.35712553492297
H	3.32316924374593	14.44688157092281	9.26208488058757
O	7.91923290009965	20.66891778475546	9.30669085273251
H	8.49541658584166	19.90428593915029	9.08170499856427
H	7.08798779754746	20.28450398958684	9.62814513018868
O	11.56917515487533	15.09794603680266	9.26722023327528
H	10.86030533815209	14.42779537947601	9.16473281672617
H	12.39560891355099	14.57739902233568	9.29189258263768
O	11.33789773211814	9.72832120559398	9.35490327864045

H	10.84586350055599	8.90740370765573	9.13808519877378
H	12.13979780341837	9.44301479930396	9.82421294023990
O	7.76697410016031	14.99722161513300	9.57685053164828
O	7.42405162942740	13.00714383940420	10.75488164004987
C	7.60200920623014	13.99490789278805	10.16357223120400

Explicitly solvated surface without CO₂

Energy=-8724.51667517733

H	-1.93139900988870	5.16831499666156	-3.18721299278646
H	-1.92298199968140	-0.27851302939548	-3.20954199360141
H	-1.91455697216833	-5.72664397563700	-3.22984401687490
H	5.78024600374158	-0.26786100156534	-3.23053100272550
H	-1.11723898004941	-10.08642197758415	-0.11890500384862
Ga	-1.89238745946324	5.82812639835286	-0.10649232868189
Ga	-1.95952524884770	0.49345733410847	-0.15661628986621
Ga	-1.94014041833871	-5.04722142915910	0.01959618767705
Ga	5.75432087706753	0.39003032519154	0.03893113991763
H	5.01967798250675	-4.63295699722127	-0.11505499481107
H	-5.77458395811092	-0.28594797342366	-3.19590100850663
H	1.92021100745745	5.17434499775551	-3.19875599132210
H	1.92862800629415	-0.27248401927507	-3.22108500763477
H	1.93705298388981	-5.72061298926208	-3.24138801460982
H	-6.91759004371161	-1.88211603249351	-2.02920198546956
H	6.93519899292833	-1.86043299813723	-2.07071799964536
Ga	0.03233907766688	3.05925690005790	-2.13552304759270
Ga	0.01687228346175	-2.38485906378076	-2.13227252617067
Ga	0.00767793224317	-7.89286773465051	-2.11909301151260
Ga	-0.00650493738199	8.51448248924340	-2.09223747959079
Ga	-3.89324344074954	3.03521211690379	-2.09785784996839
Ga	-3.87991801808681	-2.44066507515719	-2.09573897351155
H	-3.05637702862787	-7.32226302865276	-2.06289098645784
Ga	3.88339977351453	3.03687542196315	-2.11810898396835
Ga	3.89545811851387	-2.41940337664681	-2.13304080752464
H	3.09082301323918	-7.31264201440206	-2.08131398628760
Ga	-5.73071407325928	0.35578382688901	0.06485543774714
H	-4.98173598667907	-4.64861299145506	-0.08508000949833
H	1.17200499052616	-10.08283800139259	-0.12576600133496
Ga	1.90571736528195	5.80814389338173	-0.02050258795106
Ga	1.95483687931703	0.32020219795982	0.00706423900154
Ga	1.97131389981762	-5.04094012059841	-0.03232349698607
H	-6.93525398448186	-1.64096097921808	1.68167299946035
H	6.97438498608511	-1.61918799280627	1.63998799910749
Ga	0.14457134824111	3.30512536244072	1.54020794633362
Ga	0.03061729179482	-2.21838917992417	1.76748456769859
Ga	0.01695932342108	-7.53102645480725	1.58075560163714
Ga	0.00911416887906	8.74935296359079	1.65290201415932
Ga	-3.96281396267370	3.07402816094576	1.93767974630909
Ga	-3.98363004721450	-2.32083612082481	1.90386870166726
H	-3.07384500754819	-7.08113600676672	1.64835800176587
Ga	3.84890619444786	3.28911082534518	1.67569061491140

Ga	3.93877858664698	-2.19269365909225	1.76117121108361
H	3.12981400590987	-7.07142600689989	1.62976499780482
P	-1.92033650659849	4.38081803278433	-2.00869820300744
P	-1.93943253261518	-1.02336852164845	-2.00971522815559
P	-1.92198809624453	-6.45757163006221	-2.00066050912941
H	-1.32479398391660	9.40197299906904	-2.00017100054049
H	5.14853899981331	3.95158000509527	-2.04174799941106
P	5.79207923479578	-1.00707540237343	-2.00854887187200
P	-1.91088065664732	4.34354726199928	1.83768092549658
P	-1.98194690762064	-0.96645336434910	1.68693745443979
P	-1.94050930081486	-6.30693636078996	2.03880515957689
H	-1.30268599402207	9.59892500304475	1.89024500291383
H	5.15858899574441	4.15620999853844	1.84565399526510
P	5.85408685824861	-0.85388369195203	2.07901472901553
H	0.01567499980986	-8.78633200170304	-3.34998199303470
H	-0.00965300442019	7.52618600151300	-3.32297599811020
H	-0.00121500284325	2.08701599798512	-3.33435799959773
H	0.00721200071699	-3.35646597476891	-3.35157100484074
H	-3.85283800884931	2.07568601977080	-3.33017698114796
H	-3.84438701054923	-3.35853298332362	-3.33452799585194
H	3.85038199968623	2.08774499974557	-3.35326099999708
H	3.85883299962113	-3.34647398612082	-3.35761300116375
H	-5.14889998252159	3.93545998596811	-2.01088701362258
P	-5.77589908396683	-1.02869839082064	-1.97669311598925
P	1.93742928650867	4.41372132105564	-1.99956013619127
P	1.95783993755108	-1.02187680232517	-2.00928308590815
P	1.94596147803723	-6.46244152946787	-2.02208471562346
H	1.30755399157302	9.40609299882260	-2.00806000078058
H	-7.05401399619172	1.15752096884818	-0.07295800416279
H	7.07389399982361	1.17963699766801	-0.11530000021377
P	0.02810055638730	-9.24180438561060	-0.10026497140716
P	0.00777729515711	7.17597190098035	-0.08560131218732
P	0.04538218903892	1.70540144575170	-0.13473440354608
P	0.01225660176023	-3.69407030838341	-0.11710421481910
H	-3.21785799024516	6.61546799717127	-0.06255900583858
P	-3.86428192933700	1.78781651972461	-0.07397617991971
P	-3.90178633765884	-3.72324669247349	-0.05270349196686
H	3.22088599026162	6.62554799857427	-0.08185499974311
P	3.82350170319930	1.73534196472257	-0.10536519656838
P	3.92999105662787	-3.71514959926481	-0.09987546386407
H	-5.13625699696029	4.14009500151942	1.87650699793948
P	-5.82337299092520	-0.86070435696182	2.11550098515972
P	1.93672387768492	4.58800395774549	2.12468783071887
P	1.96986923659895	-0.91087078832794	2.06972854162759
P	1.99868280207482	-6.28422333659293	1.99944557679266
H	1.30818198860898	9.60301299661744	1.88242099927894
O	-3.27625905769862	-3.39665102158940	3.35087601806507
O	-0.72567962284777	-3.38282506807576	3.31452872072390
H	-2.00043146951574	-0.10442423240654	2.80277177851428

H	-3.57986501056318	-3.07515006805779	4.21457942938769
H	-1.78246451241326	-3.40766454453001	3.35023052340888
H	-0.41912412088725	-4.29666645447648	3.42682286892885
H	-1.72143815188356	5.22043052582948	2.92562845777947
O	-3.88188067034075	1.97203488995964	3.46363808123126
H	-4.41244306260981	1.17252160923736	3.32267316298945
O	0.23020687055990	7.37509628634980	3.30886243953833
H	0.80701469830975	6.61071883837499	3.08567942973321
H	-0.59749280313438	6.99064203642000	3.63930582228350
O	3.94552683316669	1.82749759783247	3.27391069200774
H	3.22202335383975	1.16946703016326	3.21894695055453
H	4.76508860711259	1.29520276014635	3.26429904024047
O	3.66621576264220	-3.56732116707832	3.37012531785834
H	3.17780650997974	-4.39066407201656	3.15466930034556
H	4.47235069827119	-3.84832991339368	3.83462346726609

3) HCOOH

HCOOH on explicitly solvated surface

Energy=-8837.7979454682

H	-1.94979000341587	5.18142199811755	-3.22929600379279
H	-1.94987900530186	-0.26526398637787	-3.27249000794296
H	-1.94996598585070	-5.71326198850845	-3.31365899782069
H	5.75334100956101	-0.26675702310262	-3.27677898173142
H	-1.16626099220627	-10.08615200649645	-0.21776300042245
Ga	-1.87864361197342	5.90793211176631	-0.21685109294280
Ga	-1.91797672789724	0.39789070068276	-0.04414265236598
Ga	-1.94563141672347	-5.05689981528568	-0.07016670314487
Ga	5.71447951166083	0.38960459473336	-0.00588502209744
H	4.97915498610073	-4.64251099443401	-0.17973199195255
H	-5.80148600539699	-0.26664000107284	-3.26720700025938
H	1.90181900408805	5.18138299678093	-3.23248700291288
H	1.90173000573496	-0.26530399148727	-3.27567903557396
H	1.90164299147483	-5.71330197986552	-3.31685101655454
H	-6.94952399612829	-1.86543699832169	-2.10911799918648
H	6.90326298921120	-1.86557998180863	-2.12059100400322
Ga	-0.00730210879928	3.04559408556797	-2.15161959124435
Ga	-0.01627015365608	-2.36849432386623	-2.21622126034803
Ga	-0.02112583906035	-7.88814115307066	-2.20547310845985
Ga	-0.01504641528820	8.53034296836196	-2.12908372476874
Ga	-3.90184441040806	3.04217640243720	-2.14657542659571
Ga	-3.88998110305511	-2.40534720080885	-2.19655915025159
H	-3.09681800294938	-7.31151399904113	-2.15531199018575
Ga	3.85234183643445	3.05295784168849	-2.16408914261494
Ga	3.85366403818404	-2.41338687174579	-2.19309163292645
H	3.05038200514800	-7.31157900760191	-2.16040398791848
Ga	-5.76683036555838	0.39613296352769	-0.00337243140728
H	-5.02225598229433	-4.64240798956038	-0.17144800332352
H	1.12298198532806	-10.08617498847941	-0.21965899454636
Ga	1.88328419132012	5.75383335536989	-0.00268508698903

Ga	1.91356191931404	0.42636696291145	-0.10648749680445
Ga	1.94309850414742	-5.05894371583921	-0.07840139886917
H	-6.97487097921982	-1.63845299524859	1.60258100041488
H	6.93476503549113	-1.63859701760910	1.59106095947241
Ga	0.01805769898261	3.08523457062017	1.84357092400867
Ga	0.04399066681399	-2.13067152634624	1.51602764795466
Ga	-0.01765444051677	-7.53664762246856	1.50061038776970
Ga	-0.01149004375981	8.74092444558366	1.61097485618561
Ga	-3.86724286168328	3.24970868459914	1.66657732612932
Ga	-3.97206285434947	-2.07928296933803	1.50156071410785
H	-3.12196903049960	-7.08455901242284	1.55676099965336
Ga	3.79574283150864	3.29238681274832	1.66003410495236
Ga	3.87168893652118	-2.16133504908313	1.65642450419512
H	3.08168803436335	-7.08462400257139	1.55162299395589
P	-1.93857038540747	4.39919345291177	-2.05643874046666
P	-1.96116244008337	-0.99945988449039	-2.04993518562453
P	-1.95583561096873	-6.45608201786144	-2.09203027367115
H	-1.33911900078454	9.40952199978333	-2.02473299734690
H	5.12568399313156	3.94908399797502	-2.07320400682466
P	5.76019132133592	-1.00998782374890	-2.05675813115260
P	-1.88103257529606	4.49269732154158	1.68229787867290
P	-1.95765106633849	-0.97351160502549	1.97135270610249
P	-1.98846594268096	-6.30567901958211	1.95339494906476
H	-1.32515499594933	9.59155500147343	1.86642199976923
H	5.12760900131364	4.13882399813630	1.81493799830592
P	5.81226475200315	-0.87230775333831	2.02655045444317
H	-0.02429600517817	-8.77551699758037	-3.44135198527670
H	-0.02406199995636	7.53673199551300	-3.35186300124573
H	-0.02414200011644	2.09766100322461	-3.38407800736990
H	-0.02422600434522	-3.34570001270856	-3.42214199723213
H	-3.87575799863501	2.09242899664830	-3.38826900141089
H	-3.87583099366375	-3.34171800101109	-3.41343599684798
H	3.82746100580648	2.09235000520560	-3.39464900369360
H	3.82738700091984	-3.34179699017019	-3.41981499058497
H	-5.17175299877200	3.94918899961920	-2.06467500329648
P	-5.80554594018680	-1.01182391752920	-2.04797207960795
P	1.90266185062663	4.41414886817974	-2.03248082669211
P	1.92446295502421	-1.00142811346708	-2.06309769442788
P	1.91258255574855	-6.45637570662057	-2.09484268467519
H	1.29322900115599	9.40949400084836	-2.02691400067771
H	-7.08542198701158	1.16689499607889	-0.14154899470356
H	7.04248291639290	1.16674998270285	-0.15325194930174
P	-0.02119055560683	-9.24273186105518	-0.18998681024109
P	0.03193817243071	7.20323739458524	-0.14685106443814
P	-0.01711173102014	1.76498324841844	-0.13235889202695
P	0.00183590567542	-3.71716449052070	-0.23719906762414
H	-3.24075200090616	6.61864400112120	-0.10193099705437
P	-3.83908627980367	1.73140615072086	-0.13215661388940
P	-3.91935998744272	-3.75005148047724	-0.17471992190851

H	3.19799200093947	6.61857900443795	-0.10726299783673
P	3.81528147207394	1.77012910562011	-0.15831739503822
P	3.89018851388217	-3.72327695219601	-0.16809675276090
H	-5.16723499402483	4.13892999511210	1.82346400204130
P	-5.87497295627838	-0.85073151259305	2.05402863141630
P	1.85353288090982	4.52308458899137	2.10228870165603
P	1.94231519217646	-0.81778669316103	1.90952804054235
P	1.95590879944282	-6.30974408136471	1.95145500392321
H	1.28571199931654	9.59152900146129	1.86425899854574
O	-0.65776576322963	1.97386487416618	3.28793752317274
H	-2.25883167094971	1.96879701275385	3.29066285667459
H	-0.39083049482230	1.04500036435159	3.19632930082731
H	-1.95264937352122	5.33155356433631	2.81513869089946
O	-3.28516427691368	2.02582710654002	3.25379945058840
H	-3.58557938562345	2.31967921234263	4.12834349714545
O	0.19967172234318	7.31408816482588	3.23208151793965
H	0.79260807756423	6.56031027984007	3.00055181436538
H	-0.64015365183763	6.90601056054350	3.49690903092907
O	3.90556553420953	1.77899588105819	3.22547322895856
H	3.20208796985904	1.10460151144110	3.11147538371046
H	4.73747853821159	1.26636173385990	3.21510598527823
O	3.31767144490006	-3.47662602954534	3.25127922439418
H	2.34708059062499	-3.59203870061179	3.32138831176473
H	3.68572311394412	-4.37593261209620	3.23878292031127
O	-1.56564289029263	-3.41719313239579	4.27981480540087
O	0.36226801489333	-3.56052755067890	3.10908358133392
C	-0.41227454173091	-3.95759245956273	3.99624981236820
H	-1.73200155346049	-2.60619894334260	3.73926054808577
H	-0.16299858068350	-4.81208834845354	4.62568726607273

Explicitly solvated surface without HCOOH

Energy=-8648.08909125077

H	5.77741512297569	18.48719920643402	2.80454891655951
H	5.77741495865144	13.04046340947657	2.76833015933443
H	5.77741483136395	7.59242002554471	2.73413667056618
H	13.48063514349556	13.03905256367911	2.77042342320217
H	6.55859726956974	3.22350847822316	5.83627544012743
Ga	5.84618992887002	19.21857418421062	5.81316731145037
Ga	5.79558319457591	13.71238216806209	6.00049267599676
Ga	5.75835641943806	8.24535840281499	5.97799129226593
Ga	13.44078847625263	13.69979558464382	6.03419039622170
H	12.70392630908958	8.66726169098684	5.87242514510757
H	1.92580499115392	13.03905185549811	2.77042455608455
H	9.62902516977933	18.48719930772653	2.80454880107586
H	9.62902503252084	13.04046305041815	2.76833081524862
H	9.62902488410852	7.59242102211439	2.73413536266976
H	0.77682469021454	11.44172598037216	3.92960755212161
H	14.62961383291626	11.44172606619592	3.92960799478200

Ga	7.72520234476331	16.34620409795787	3.89241389070718
Ga	7.70368432373072	10.94373920289478	3.82639325630101
Ga	7.69799165948580	5.41062678735915	3.85247125569266
Ga	7.71131377159030	21.83809323890090	3.90157753023946
Ga	3.82470561833544	16.35175611952927	3.88615269057187
Ga	3.83386304921818	10.90319983342008	3.84443597142975
H	4.62962038405205	5.99564064482114	3.89357730485115
Ga	11.57654046302512	16.35680055958451	3.88125397952156
Ga	11.58192606749255	10.89823807207172	3.84955229433094
H	10.77682047546331	5.99563924331829	3.89357709357281
Ga	1.95700467469243	13.70516445705917	6.03735570635293
H	2.70251344766828	8.66726135180146	5.87242545052007
H	8.84784143871863	3.22350890016492	5.83627574204294
Ga	9.60761416137981	19.06518547498991	6.03434749262458
Ga	9.64040204755992	13.71327227725546	5.96913229450541
Ga	9.67771321121766	8.24429071923326	5.94573816695837
H	0.74840066187756	11.67346247508620	7.64098895565286
H	14.65803969806814	11.67346265119954	7.64098962244284
Ga	7.73856000055315	16.40028762458186	7.88576059030545
Ga	7.71463829270370	11.23133549936621	7.48523897722419
Ga	7.69439323607572	5.79077153174819	7.57375238313972
Ga	7.71151501635875	22.05335786801867	7.64233811768726
Ga	3.85603621891703	16.56493079913672	7.70308635178638
Ga	3.75485007220995	11.23244025150675	7.55952959260210
H	4.60139087023573	6.22734724226721	7.60533347618184
Ga	11.51747524762419	16.60801578419111	7.70913882380182
Ga	11.63150638686324	11.11689835915198	7.71354204677605
H	10.80504969690445	6.22734637135445	7.60533301239090
P	5.79101809868604	17.70405276516771	3.97849746237278
P	5.76099278021145	12.31306109716923	3.99371272160022
P	5.76925357114485	6.85044208448272	3.95641086700208
H	6.38704564584651	22.71684345985823	4.00420320865320
H	12.85194060139963	17.25642354712872	3.96807757143052
P	13.48734841102551	12.29792681170521	3.99012612184153
P	5.84211890213444	17.80709699238255	7.71370978812388
P	5.75574115304955	12.36474151465259	8.02599499622518
P	5.72025082007504	7.01824012767200	8.01208696403238
H	6.39778594308948	22.90385779750725	7.89512876587065
H	12.85064299683100	17.45114199148705	7.85597216093596
P	13.53991066426175	12.44867013250641	8.06691087623847
H	7.70321980498188	4.53002827941741	2.61196076213136
H	7.70321997381243	20.84237173149993	2.68056187744381
H	7.70322005060629	15.40326651940942	2.65531102960492
H	7.70321993606806	9.95986308838373	2.62421712737304
H	3.85161010948411	15.39798389602676	2.64793613199969
H	3.85160996454226	9.96381133757839	2.62972787223357
H	11.55483006291023	15.39798440646758	2.64793741378317
H	11.55482988254622	9.96381195950937	2.62972858941776
H	2.55450141174129	17.25642186440939	3.96807768169006

P	1.91962056387132	12.29683802590554	3.99133096845693
P	9.62964991142300	17.72194251804661	4.00673520720991
P	9.64999412775646	12.30485810688594	3.98596085362684
P	9.63440374002480	6.84341710217920	3.94982711425030
H	9.01939440334284	22.71684272022532	4.00420262654630
H	0.63926648867020	14.47657187824051	5.89317729049559
H	14.76717412814347	14.47657320619406	5.89317634227245
P	7.70415992115753	4.07032620122340	5.87577830022246
P	7.75655518293407	20.51372654092834	5.88604962585609
P	7.71294822097794	15.06212307667420	5.91867811641151
P	7.71894040661568	9.56933153421809	5.81801200563473
H	4.48384898383680	19.92840928013227	5.92900072502092
P	3.88037791726420	15.04817066690625	5.90313582209218
P	3.79978590263763	9.56697274388387	5.87081325855207
H	10.92259260961000	19.92841058831850	5.92900143104711
P	11.53438728958314	15.07040033959960	5.89902143744544
P	11.61858931430551	9.58666215789375	5.87348905612956
H	2.55579673154194	17.45114106780121	7.85597165532189
P	1.84512432630054	12.46301761203540	8.09510419041518
P	9.57473362679164	17.83790616130716	8.14186493191145
P	9.66588079635654	12.41188903923785	8.00664340078314
P	9.68600880374023	7.02127906869031	7.98644293365607
H	9.00865295827501	22.90385826116177	7.89512906847552
O	7.05999684047596	15.31275990246080	9.34687155004436
H	5.45996848160020	15.30122577002694	9.34213444643556
H	7.32165121701726	14.38068200763785	9.27474612216797
H	5.77395144670513	18.64648915874329	8.84597043783475
O	4.43350135286066	15.34871435476881	9.29446919023696
H	4.11976684300253	15.63684465479256	10.16615474843691
O	7.91972412257218	20.63156160449239	9.26756076345698
H	8.51135772810377	19.87602860031986	9.03920392972597
H	7.07941307969264	20.22623918307331	9.53505644673441
O	11.63387237738401	15.10574058680555	9.28605771909002
H	10.92168797506753	14.43889549238908	9.20227728662292
H	12.46081520734794	14.58540280356107	9.27119199882285
O	11.52237563843617	9.64305777900603	9.25294090632348
H	11.33491739624056	9.97841851347628	10.14590478643275
H	10.88715116125870	8.91151233016332	9.09736767333129

4) H₂O

H₂O on explicitly solvated surface

Energy=-8801.00780384292

H	5.77741512946523	18.48719920334192	2.80454892802419
H	5.77741493771896	13.04046341748800	2.76833020940921
H	5.77741493582684	7.59242009080566	2.73413664926354
H	13.48063509614932	13.03905259513365	2.77042343987939
H	6.55859737068989	3.22350849600713	5.83627543511794
Ga	5.82195892378414	19.14323312227681	5.95469463912361
Ga	5.75875047751927	13.85161504991147	5.81653109985324

Ga	5.73799667437690	8.27090268539008	5.98575683323883
Ga	13.43595300181289	13.69759652912622	6.03672212356016
H	12.70392629006523	8.66726174870932	5.87242507923351
H	1.92580495603947	13.03905183921299	2.77042456841676
H	9.62902520508861	18.48719931618661	2.80454880375853
H	9.62902505213948	13.04046307091293	2.76833079271069
H	9.62902483716757	7.59242104534154	2.73413536668939
H	0.77682475021011	11.44172601980651	3.92960754908917
H	14.62961388699484	11.44172602638451	3.92960798678121
Ga	7.71891162333673	16.37093203113892	3.87589577302775
Ga	7.70552025670846	10.94173864265487	3.83925033920796
Ga	7.69153562654074	5.42244522275834	3.84461349749277
Ga	7.70808524615561	21.82427664445399	3.91637203867775
Ga	3.82948373491265	16.36093367572789	3.88994750634845
Ga	3.81016071710702	10.89388259085808	3.86634099158841
H	4.62962025349697	5.99564054025928	3.89357731034717
Ga	11.56905419637403	16.35112172569976	3.89104247287649
Ga	11.57196765231514	10.89872589825580	3.85651710392135
H	10.77682055698953	5.99563918287274	3.89357707702485
Ga	1.98649128003947	13.71714739176976	6.08669365553230
H	2.70251343863900	8.66726133426755	5.87242543634921
H	8.84784134010362	3.22350893195217	5.83627573130795
Ga	9.59797717843332	19.08830243556881	6.03990432576223
Ga	9.58981506097433	13.69506338488623	6.00903753733804
Ga	9.65690326535687	8.26477369758920	5.94220918518140
H	0.74840065151308	11.67346249523235	7.64098896832396
H	14.65803972140373	11.67346263523218	7.64098961178853
Ga	7.60366797526134	16.62519239149813	7.74803965846104
Ga	7.70495637764936	11.07436819760535	7.71928173791864
Ga	7.69087320096222	5.77667190195518	7.54368062385561
Ga	7.70417543810994	22.03355663684580	7.64276468344303
Ga	3.96313763736714	16.62402647173247	7.82255706745486
Ga	3.68835641271886	10.99420294135379	7.86360394823334
H	4.60139091691730	6.22734726714756	7.60533347605673
Ga	11.51104098103212	16.60294180827303	7.68373991835989
Ga	11.60281940146291	11.12566349066790	7.74544431796689
H	10.80504966937009	6.22734636278315	7.60533301483139
P	5.78646655989396	17.72198736217528	3.99807505959451
P	5.75316392890630	12.30487296272956	3.97293539130773
P	5.76370603135206	6.85997952311086	3.96284020622569
H	6.38704549429970	22.71684348158485	4.00420321751759
H	12.85194059544033	17.25642353383720	3.96807752977816
P	13.48512601470533	12.29546424490870	3.99028564607164
P	5.80829311007192	18.06373658784559	8.04074915362942
P	5.69538908550851	12.31528980392421	7.61358205016442
P	5.73366944517259	7.00053786961778	8.00076639568458
H	6.39778624299326	22.90385787254886	7.89512873230490
H	12.85064299618835	17.45114200890303	7.85597216908941
P	13.53529017870911	12.44169741234886	8.07353705298446

H	7.70321979990249	4.53002828055966	2.61196078974130
H	7.70322007613260	20.84237175151169	2.68056192039909
H	7.70322004563375	15.40326649080262	2.65531097571647
H	7.70321993294971	9.95986304882621	2.62421707586976
H	3.85161004107265	15.39798402902952	2.64793623816795
H	3.85160997941188	9.96381132570328	2.62972788968780
H	11.55483006430310	15.39798443422358	2.64793744939046
H	11.55482989324315	9.96381196084919	2.62972870940959
H	2.55450151459281	17.25642176046385	3.96807761840359
P	1.91440381484574	12.30960084030064	4.00263080828165
P	9.63129449918924	17.73034904029024	4.00928692597813
P	9.64194868274987	12.31072710691022	3.99343709118424
P	9.63350688487806	6.84688876661651	3.95136568649002
H	9.01939443241809	22.71684272484559	4.00420261732917
H	0.63926640146676	14.47657189399024	5.89317725944620
H	14.76717409237738	14.47657318761346	5.89317634374049
P	7.70511187569435	4.06676530897424	5.86025006841062
P	7.72590337282746	20.50017197938940	5.88342848701352
P	7.71248646194485	15.11356783844257	5.90428147251189
P	7.70038045210139	9.60477925136622	5.84222275129815
H	4.48384900589519	19.92840927237843	5.92900072120730
P	3.85273446008266	15.14304976100114	5.92432868734797
P	3.77783698700441	9.59526410164066	5.90563363699973
H	10.92259256157590	19.92841054818793	5.92900143593212
P	11.51308102133620	15.04016704082214	5.90048613653458
P	11.61461887487308	9.59027160490375	5.88627150613456
H	2.55579679469749	17.45114103872225	7.85597165679632
P	1.84845736139687	12.45081160094124	8.11111252864839
P	9.58418919871589	17.83882103893039	8.13369749594241
P	9.62487764340268	12.40254763197292	8.05313066245090
P	9.67424011086676	7.01629693057552	7.97223198203790
H	9.00865266198256	22.90385814319700	7.89512903136801
O	4.39347178159172	9.90335298805584	9.30683717273643
O	6.94051447783615	9.92579511736982	9.28088293534880
H	5.64955831568575	13.11916059756585	8.76663895714107
H	4.09769305167613	10.24114388040942	10.16711187577979
H	5.88134191747317	9.89510908638013	9.30672127805033
H	7.25340664414515	9.01681012913568	9.41228808398000
O	4.44825659481993	15.27568568205692	9.21028552683735
O	6.96685850117719	15.28334545951606	9.23840177767386
H	4.15512404945554	15.56150436767613	10.08957278233589
H	5.89367133815420	15.24666941270371	9.24938010518154
H	7.32065995714287	14.38133010672023	9.20174624330820
O	7.71301160382398	20.53807059388983	9.23091933943887
H	8.50113391959262	19.96008340814554	9.12715366237351
H	6.96828133614213	19.90764334827930	9.05854521537313
O	11.65004362668494	15.10977538930742	9.28395870309070
H	10.93055258885098	14.44917748455847	9.21912000890029
H	12.47056149691580	14.58026154057591	9.24914037267878

O	11.32344490160228	9.74325701112381	9.35360215203224
H	10.83750793695560	8.92033379902725	9.13161495549787
H	12.13011708447910	9.46011066511247	9.81579948019167

Explicitly solvated surface without H₂O

Energy=-8724.51667517733

H	-1.93139900988870	5.16831499666156	-3.18721299278646
H	-1.92298199968140	-0.27851302939548	-3.20954199360141
H	-1.91455697216833	-5.72664397563700	-3.22984401687490
H	5.78024600374158	-0.26786100156534	-3.23053100272550
H	-1.11723898004941	-10.08642197758415	-0.11890500384862
Ga	-1.89238745946324	5.82812639835286	-0.10649232868189
Ga	-1.95952524884770	0.49345733410847	-0.15661628986621
Ga	-1.94014041833871	-5.04722142915910	0.01959618767705
Ga	5.75432087706753	0.39003032519154	0.03893113991763
H	5.01967798250675	-4.63295699722127	-0.11505499481107
H	-5.77458395811092	-0.28594797342366	-3.19590100850663
H	1.92021100745745	5.17434499775551	-3.19875599132210
H	1.92862800629415	-0.27248401927507	-3.22108500763477
H	1.93705298388981	-5.72061298926208	-3.24138801460982
H	-6.91759004371161	-1.88211603249351	-2.02920198546956
H	6.93519899292833	-1.86043299813723	-2.07071799964536
Ga	0.03233907766688	3.05925690005790	-2.13552304759270
Ga	0.01687228346175	-2.38485906378076	-2.13227252617067
Ga	0.00767793224317	-7.89286773465051	-2.11909301151260
Ga	-0.00650493738199	8.51448248924340	-2.09223747959079
Ga	-3.89324344074954	3.03521211690379	-2.09785784996839
Ga	-3.87991801808681	-2.44066507515719	-2.09573897351155
H	-3.05637702862787	-7.32226302865276	-2.06289098645784
Ga	3.88339977351453	3.03687542196315	-2.11810898396835
Ga	3.89545811851387	-2.41940337664681	-2.13304080752464
H	3.09082301323918	-7.31264201440206	-2.08131398628760
Ga	-5.73071407325928	0.35578382688901	0.06485543774714
H	-4.98173598667907	-4.64861299145506	-0.08508000949833
H	1.17200499052616	-10.08283800139259	-0.12576600133496
Ga	1.90571736528195	5.80814389338173	-0.02050258795106
Ga	1.95483687931703	0.32020219795982	0.00706423900154
Ga	1.97131389981762	-5.04094012059841	-0.03232349698607
H	-6.93525398448186	-1.64096097921808	1.68167299946035
H	6.97438498608511	-1.61918799280627	1.63998799910749
Ga	0.14457134824111	3.30512536244072	1.54020794633362
Ga	0.03061729179482	-2.21838917992417	1.76748456769859
Ga	0.01695932342108	-7.53102645480725	1.58075560163714
Ga	0.00911416887906	8.74935296359079	1.65290201415932
Ga	-3.96281396267370	3.07402816094576	1.93767974630909
Ga	-3.98363004721450	-2.32083612082481	1.90386870166726
H	-3.07384500754819	-7.08113600676672	1.64835800176587
Ga	3.84890619444786	3.28911082534518	1.67569061491140
Ga	3.93877858664698	-2.19269365909225	1.76117121108361

H	3.12981400590987	-7.07142600689989	1.62976499780482
P	-1.92033650659849	4.38081803278433	-2.00869820300744
P	-1.93943253261518	-1.02336852164845	-2.00971522815559
P	-1.92198809624453	-6.45757163006221	-2.00066050912941
H	-1.32479398391660	9.40197299906904	-2.00017100054049
H	5.14853899981331	3.95158000509527	-2.04174799941106
P	5.79207923479578	-1.00707540237343	-2.00854887187200
P	-1.91088065664732	4.34354726199928	1.83768092549658
P	-1.98194690762064	-0.96645336434910	1.68693745443979
P	-1.94050930081486	-6.30693636078996	2.03880515957689
H	-1.30268599402207	9.59892500304475	1.89024500291383
H	5.15858899574441	4.15620999853844	1.84565399526510
P	5.85408685824861	-0.85388369195203	2.07901472901553
H	0.01567499980986	-8.78633200170304	-3.34998199303470
H	-0.00965300442019	7.52618600151300	-3.32297599811020
H	-0.00121500284325	2.08701599798512	-3.33435799959773
H	0.00721200071699	-3.35646597476891	-3.35157100484074
H	-3.85283800884931	2.07568601977080	-3.33017698114796
H	-3.84438701054923	-3.35853298332362	-3.33452799585194
H	3.85038199968623	2.08774499974557	-3.35326099999708
H	3.85883299962113	-3.34647398612082	-3.35761300116375
H	-5.14889998252159	3.93545998596811	-2.01088701362258
P	-5.77589908396683	-1.02869839082064	-1.97669311598925
P	1.93742928650867	4.41372132105564	-1.99956013619127
P	1.95783993755108	-1.02187680232517	-2.00928308590815
P	1.94596147803723	-6.46244152946787	-2.02208471562346
H	1.30755399157302	9.40609299882260	-2.00806000078058
H	-7.05401399619172	1.15752096884818	-0.07295800416279
H	7.07389399982361	1.17963699766801	-0.11530000021377
P	0.02810055638730	-9.24180438561060	-0.10026497140716
P	0.00777729515711	7.17597190098035	-0.08560131218732
P	0.04538218903892	1.70540144575170	-0.13473440354608
P	0.01225660176023	-3.69407030838341	-0.11710421481910
H	-3.21785799024516	6.61546799717127	-0.06255900583858
P	-3.86428192933700	1.78781651972461	-0.07397617991971
P	-3.90178633765884	-3.72324669247349	-0.05270349196686
H	3.22088599026162	6.62554799857427	-0.08185499974311
P	3.82350170319930	1.73534196472257	-0.10536519656838
P	3.92999105662787	-3.71514959926481	-0.09987546386407
H	-5.13625699696029	4.14009500151942	1.87650699793948
P	-5.82337299092520	-0.86070435696182	2.11550098515972
P	1.93672387768492	4.58800395774549	2.12468783071887
P	1.96986923659895	-0.91087078832794	2.06972854162759
P	1.99868280207482	-6.28422333659293	1.99944557679266
H	1.30818198860898	9.60301299661744	1.88242099927894
O	-3.27625905769862	-3.39665102158940	3.35087601806507
O	-0.72567962284777	-3.38282506807576	3.31452872072390
H	-2.00043146951574	-0.10442423240654	2.80277177851428
H	-3.57986501056318	-3.07515006805779	4.21457942938769

H	-1.78246451241326	-3.40766454453001	3.35023052340888
H	-0.41912412088725	-4.29666645447648	3.42682286892885
H	-1.72143815188356	5.22043052582948	2.92562845777947
O	-3.88188067034075	1.97203488995964	3.46363808123126
H	-4.41244306260981	1.17252160923736	3.32267316298945
O	0.23020687055990	7.37509628634980	3.30886243953833
H	0.80701469830975	6.61071883837499	3.08567942973321
H	-0.59749280313438	6.99064203642000	3.63930582228350
O	3.94552683316669	1.82749759783247	3.27391069200774
H	3.22202335383975	1.16946703016326	3.21894695055453
H	4.76508860711259	1.29520276014635	3.26429904024047
O	3.66621576264220	-3.56732116707832	3.37012531785834
H	3.17780650997974	-4.39066407201656	3.15466930034556
H	4.47235069827119	-3.84832991339368	3.83462346726609

5) o-DHP

o-DHP on explicitly solvated surface

Energy=-8973.87938281653

H	5.77741510169305	18.48719919643186	2.80454893717634
H	5.77741494656483	13.04046339378817	2.76833019752479
H	5.77741493856184	7.59242009584685	2.73413664969039
H	13.48063509152794	13.03905258498593	2.77042345271309
H	6.55859731426614	3.22350848608381	5.83627542786245
Ga	5.84378656540901	19.20577814686484	5.82371546165591
Ga	5.77379757565861	13.72050280478456	5.88300768835580
Ga	5.73717067702423	8.28715666615762	5.98744090770626
Ga	13.43688801598538	13.70532654238322	6.03709889627163
H	12.70392630316001	8.66726173896132	5.87242508418950
H	1.92580496574505	13.03905184418445	2.77042456490146
H	9.62902516938153	18.48719931816894	2.80454881736021
H	9.62902504577180	13.04046305912269	2.76833079382893
H	9.62902483931379	7.59242105348405	2.73413535906708
H	0.77682473975448	11.44172601021702	3.92960755299122
H	14.62961388039856	11.44172603374388	3.92960798710149
Ga	7.72653097640301	16.34533790362849	3.89452295689594
Ga	7.71150014754951	10.92374241024457	3.85569543385107
Ga	7.68999522578475	5.42256036082834	3.84531353754044
Ga	7.71059775820909	21.83527375757191	3.90461185244138
Ga	3.82107757345967	16.35368264727515	3.88317239988688
Ga	3.81008463279618	10.88699324441694	3.85895472728108
H	4.62962025467028	5.99564053817670	3.89357731087539
Ga	11.57806790566515	16.35528305771239	3.88160743499088
Ga	11.58613364971467	10.89621565505821	3.85133078571649
H	10.77682055588660	5.99563918315517	3.89357708263432
Ga	1.95321544556715	13.67698482030516	6.04438924698094
H	2.70251343416541	8.66726132837949	5.87242543726791
H	8.84784139512788	3.22350891376792	5.83627573943496
Ga	9.60773763533716	19.06136686162413	6.03366904513894
Ga	9.63189273930112	13.68634808319093	5.95124938935770

Ga	9.65584880421679	8.26781242954545	5.94145632251435
H	0.74840065284993	11.67346249662655	7.64098897296803
H	14.65803971928628	11.67346263678912	7.64098961752580
Ga	7.74691605372731	16.36455124131913	7.88642168012897
Ga	7.78751836657582	11.12452732526305	7.77477081573365
Ga	7.68705904602065	5.78377772948280	7.54571236392464
Ga	7.71137244994147	22.05225599273579	7.64169133875042
Ga	3.85230887159858	16.54953558182265	7.69462305352255
Ga	3.53866706902944	10.89934988963204	7.88414505809772
H	4.60139090759347	6.22734726396930	7.60533347781144
Ga	11.51755658957913	16.59617523561471	7.70185335687185
Ga	11.63694383897743	11.13537116425717	7.71693443116983
H	10.80504967915706	6.22734637022389	7.60533301733498
P	5.79020908059438	17.70191509382548	3.97797412404792
P	5.75555839950880	12.28292955184892	3.96430060934464
P	5.76372533597173	6.86392886219345	3.96481111932830
H	6.38704555681815	22.71684347297939	4.00420321402673
H	12.85194061901262	17.25642355060918	3.96807754672062
P	13.48855687561692	12.29913843484649	3.99163602979901
P	5.84763279704353	17.77608295350903	7.72329111949818
P	5.65643403442478	12.17158224975463	7.70718470557226
P	5.72877223320048	7.01197889968645	7.99590291532352
H	6.39778616315029	22.90385783614463	7.89512872962795
H	12.85064297401053	17.45114198610605	7.85597215783973
P	13.54863402952789	12.45386740046190	8.07521614751412
H	7.70321979436914	4.53002828335937	2.61196079247542
H	7.70322005023240	20.84237176107705	2.68056191753639
H	7.70322005475893	15.40326648858124	2.65531098056485
H	7.70321993785933	9.95986305877029	2.62421706704040
H	3.85161006238438	15.39798400818376	2.64793622925165
H	3.85160997374705	9.96381133248943	2.62972787911455
H	11.55483005287602	15.39798440988988	2.64793743660128
H	11.55482989024524	9.96381195173138	2.62972868727917
H	2.55450149529526	17.25642178051682	3.96807762726683
P	1.91701789139196	12.29793661864897	3.98963011447132
P	9.63077236894572	17.72081484149895	4.00581939646635
P	9.65077633485087	12.29448694513903	3.97765352170281
P	9.63288523713450	6.84766211561648	3.95168290514723
H	9.01939439144536	22.71684270083382	4.00420261638714
H	0.63926642331466	14.47657188959891	5.89317725863886
H	14.76717412726573	14.47657320881844	5.89317634342411
P	7.70471208024378	4.06807882647722	5.86296094488809
P	7.75299511054550	20.50762408711811	5.88944205921639
P	7.70700957223290	15.04243530435194	5.91064130472621
P	7.71035684033530	9.62538020781320	5.89180202745978
H	4.48384898091272	19.92840928127161	5.92900073310927
P	3.86206271321762	15.04853101021839	5.88627582372888
P	3.76892292632690	9.60176853490660	5.88461851357991
H	10.92259267292595	19.92841062195447	5.92900143030590

P	11.52391083764492	15.06414012033639	5.88864801809772
P	11.61697308385108	9.59003358205018	5.87693749748252
H	2.55579672009549	17.45114106950163	7.85597165189312
P	1.82901740410689	12.49287716758719	8.08137998597183
P	9.57042678738646	17.82236424250727	8.13657985222187
P	9.69685415655943	12.46270552828329	7.99805620197293
P	9.67566473742260	7.01913387408968	7.97007354666602
H	9.00865274697082	22.90385817891530	7.89512904162706
O	3.39011199207870	9.52799985545503	9.16094705832708
H	5.66728786078293	13.06014285680617	8.79574757837008
H	3.29703970978274	9.89886356222539	10.05067432333853
H	5.78596513447463	18.61393091868806	8.85794872827496
O	4.46345090724349	15.27127632662828	9.24723333449056
H	4.07847405924334	15.42227391263835	10.12362116520512
O	7.91761105560825	20.62872483141323	9.26758235809023
H	8.50633536963743	19.87193030014452	9.03672614547875
H	7.07572699705355	20.22558756500721	9.53349625543654
O	11.55472133744730	15.05374118272681	9.25125434627064
H	10.89037456022268	14.35210121493606	9.06214567649249
H	12.40423542027009	14.57524148038369	9.30436259276088
O	11.41704421782757	9.71459984833899	9.29521040877467
H	10.94543815521311	8.88125713253956	9.08483288564196
H	12.21969080208891	9.46105789894860	9.78015276644976
O	7.07426795191960	15.27126216700311	9.36454021103818
H	5.48631469385164	15.25051252601398	9.34074854816727
H	7.47574009014361	14.39094782556848	9.43431500838145
C	5.80800200745049	11.07376615424341	10.82445600893139
C	6.22542430287646	10.01126218784535	10.11650244180207
C	8.52412035065904	10.53318052269106	10.69048908730205
C	8.06070079698236	11.92218200143065	11.05605495537989
C	6.73876934169803	12.15479475906555	11.14376834100057
H	6.34829152946325	13.12498249858845	11.43579499608177
H	8.80393993110120	12.67437979977599	11.29208758569942
H	8.49426735459403	9.87608106005206	11.57124075101263
H	5.57394783279583	9.23023451685746	9.74779844033834
H	4.76649224072407	11.14960366820176	11.11443240335661
N	7.59713120110266	9.96802830797573	9.65670340967112
H	7.85940863594672	8.99897967464514	9.46939056041590
H	9.53385815086452	10.53140615962609	10.28432005384619

Explicitly solvated surface without o-DHP

Energy=-8724.51547648238

H	5.77741509747177	18.48719919775901	2.80454891883170
H	5.77741495146293	13.04046339435635	2.76833018954840
H	5.77741494155768	7.59242009927257	2.73413664929510
H	13.48063509259474	13.03905258541154	2.77042345251751
H	6.55859731567273	3.22350848743840	5.83627542765242
Ga	5.84508107291889	19.21394324984356	5.81835071374590
Ga	5.77518784333971	13.73715909111388	5.89087322060488

Ga	5.71283304616836	8.27249737844637	5.99945870370818
Ga	13.44312534365783	13.69617906862570	6.03892086411457
H	12.70392630513907	8.66726172969685	5.87242508379907
H	1.92580497338914	13.03905184750453	2.77042456500826
H	9.62902517455227	18.48719932000220	2.80454880542824
H	9.62902504068255	13.04046306443398	2.76833079669220
H	9.62902483834664	7.59242105609643	2.73413535758498
H	0.77682473017076	11.44172600603859	3.92960755309745
H	14.62961387576011	11.44172603680347	3.92960798840439
Ga	7.72521279628336	16.35335792843510	3.88619319633619
Ga	7.71337566221005	10.94212500044808	3.82636049456578
Ga	7.68789086075870	5.41547004102829	3.85137887034019
Ga	7.71079193775712	21.83761520760925	3.90207472571731
Ga	3.82091888293109	16.35363869451191	3.88214748446001
Ga	3.80699624381422	10.87926004891554	3.86879085458557
H	4.62962025053145	5.99564053467291	3.89357731180842
Ga	11.57822042463714	16.35809817675193	3.87860074323662
Ga	11.59017034505889	10.89514519358143	3.85055033678897
H	10.77682055717075	5.99563918232808	3.89357708485497
Ga	1.94981351572919	13.67029562807193	6.04605303083858
H	2.70251343304720	8.66726132745492	5.87242543727253
H	8.84784139449886	3.22350891445545	5.83627573959928
Ga	9.60734904800290	19.06710354193864	6.03238228182112
Ga	9.64100795956301	13.72412960043910	5.94832320851005
Ga	9.68060113331565	8.24360581250173	5.94347457460532
H	0.74840065216925	11.67346249730513	7.64098897243269
H	14.65803971838318	11.67346263798038	7.64098961881841
Ga	7.74427883522229	16.39530952773483	7.88255062072226
Ga	7.82867662997293	11.21574770974909	7.50507244960753
Ga	7.68448259343074	5.79641359866826	7.55885213206275
Ga	7.71124671436463	22.05325934876701	7.64461437589526
Ga	3.85321946976355	16.55553548761178	7.69976363258632
Ga	3.56527272096041	10.91228323498790	7.94176287131827
H	4.60139090747981	6.22734726388498	7.60533347782984
Ga	11.51899171759688	16.61091485270230	7.70808572507729
Ga	11.63616115729244	11.12086418416221	7.72876741470096
H	10.80504968068378	6.22734637010931	7.60533301732756
P	5.78879063162661	17.70408924155392	3.97841876047059
P	5.75321610191577	12.28663366105423	3.97064045768815
P	5.76243604339409	6.86327871915358	3.96567045497024
H	6.38704577629284	22.71684345247440	4.00420319396951
H	12.85194063964700	17.25642357847312	3.96807756964499
P	13.48923594332359	12.29922264802803	3.99103349640390
P	5.84148760746033	17.79115132376608	7.71810623232353
P	5.69978539534084	12.17565759812449	7.75520437333998
P	5.71823185745615	7.02001562505316	8.01782038234388
H	6.39778569828277	22.90385774673541	7.89512879131206
H	12.85064300389107	17.45114199495385	7.85597216467311
P	13.54539375682829	12.44801514557655	8.07842116054714

H	7.70321979422935	4.53002828098938	2.61196079156684
H	7.70321988376545	20.84237171648082	2.68056184125586
H	7.70322005389729	15.40326648345500	2.65531097525534
H	7.70321993798093	9.95986305860163	2.62421707101641
H	3.85161008563805	15.39798396248297	2.64793619141775
H	3.85160997027179	9.96381133464324	2.62972787873943
H	11.55483003978755	15.39798437799332	2.64793740646785
H	11.55482989338770	9.96381194418206	2.62972868079784
H	2.55450146067764	17.25642181300735	3.96807765211522
P	1.91743635179980	12.29698457808444	3.98948860482879
P	9.63112048114869	17.72260766487037	4.00651863349116
P	9.65551718453972	12.30250727303634	3.98350045409491
P	9.63231808668816	6.84263834763547	3.94879538815047
H	9.01939438499578	22.71684272530170	4.00420263966765
H	0.63926643584369	14.47657188120900	5.89317726117006
H	14.76717412943120	14.47657320971811	5.89317634473225
P	7.70416398299378	4.06994872762131	5.87223033705804
P	7.75430034768350	20.51168988701113	5.88862161124025
P	7.70744924380139	15.05883613160127	5.91140568571259
P	7.71443250621640	9.57584948191682	5.82709769439137
H	4.48384900547417	19.92840926220835	5.92900072967535
P	3.85795572614203	15.04895840814550	5.89300280022838
P	3.76373724825697	9.61119057616081	5.91555933578660
H	10.92259263320683	19.92841059753119	5.92900142951249
P	11.53788200231999	15.07249802102310	5.89833380255121
P	11.61959123655018	9.59146070888638	5.87758158880048
H	2.55579667508672	17.45114109245613	7.85597166644984
P	1.83006882435157	12.48778082190822	8.08587215453369
P	9.57430035149541	17.83523564987819	8.13847772826090
P	9.69617367164199	12.46560772921433	8.02016741631284
P	9.68243758175966	7.02082518122202	7.98021642859335
H	9.00865319001352	22.90385835153764	7.89512909374752
O	3.66242938843909	9.69014370077828	9.35110891963734
O	7.07276619788762	15.30860978106969	9.35299467245544
H	3.25985190481177	10.10152849601493	10.13162241360748
H	5.48463977104196	15.27024216454073	9.33828823888328
H	7.50013269474339	14.44287423911900	9.43881244959072
H	5.77961883982561	18.62721214501111	8.85290914673755
O	4.46158208425750	15.28054026903455	9.24546846360233
H	4.08611910955084	15.44052002315355	10.12508187445341
O	7.91559081290215	20.63239567754277	9.27022967941281
H	8.50598998112333	19.87565352232183	9.04445015801504
H	7.07440554358786	20.22979522092129	9.53903498875145
O	11.66848020003279	15.13519385643012	9.29621101106272
H	10.94716290649625	14.47578854376110	9.26623435981056
H	12.48888822517922	14.60493277929182	9.27053655568958
O	11.30551078133284	9.76526326230245	9.33345137367537
H	10.77684826658162	8.96403794359265	9.12595889674433
H	12.10043589234984	9.45041578440713	9.79557499720549

H	5.83231404269017	13.06495980365763	8.83768399994404
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6) Py

Py on explicitly solvated surface

Energy=-8972.70466424681

H	-1.90321599385620	5.13165004903907	-3.39153004008579
H	-1.92283400183362	-0.31530699845622	-3.39458501078025
H	-1.94244901584813	-5.76355798846171	-3.39560600914928
H	5.78038898336617	-0.34425495377284	-3.42190003955106
H	-1.16504506682481	-10.11637497799414	-0.26984901365727
Ga	-1.85412953502147	5.79483844530466	-0.30219145043362
Ga	-1.91728241502560	0.48382353540946	-0.33787319765790
Ga	-1.96485280395931	-5.06622662664302	-0.14537703517958
Ga	5.75581044509030	0.32845766093068	-0.15756134917578
H	4.99989100390632	-4.69437999702271	-0.29031299550122
H	-5.77444099632829	-0.30293099620149	-3.37777399869456
H	1.94839409062832	5.11787505363049	-3.40623889352253
H	1.92877599998855	-0.32908199947161	-3.40929201203657
H	1.90916092661094	-5.77733193566963	-3.41031602394492
H	-6.92470700575609	-1.88908900206534	-2.20447599890278
H	6.92808202171383	-1.93863303428408	-2.25737697803388
Ga	0.05108689685665	2.99771208135178	-2.29834527995903
Ga	0.00585891303197	-2.42376012293334	-2.31339945845566
Ga	-0.03341704874452	-7.93494532532155	-2.27886199917879
Ga	0.04101713721072	8.46724580846760	-2.30528261741319
Ga	-3.87074808334713	3.01095468008800	-2.28848379029561
Ga	-3.88965198230044	-2.45657892148025	-2.27082499169415
H	-3.09152700907139	-7.34917300239199	-2.22206000162320
Ga	3.89505223366639	2.97837910663712	-2.32107160816753
Ga	3.87680378840875	-2.47590271678628	-2.31646716491582
H	3.05567408527178	-7.37116007378607	-2.24553497462420
Ga	-5.72731920941532	0.34526772805615	-0.08322613072927
H	-5.00152199390546	-4.65861099198605	-0.25211999858763
H	1.12419907629733	-10.12456303155227	-0.27859099177023
Ga	1.94228074880304	5.73949981359610	-0.21726465668883
Ga	1.92693713486080	0.29868776200724	-0.17473662346397
Ga	1.95076156130265	-5.09084840719920	-0.20745190063687
H	-6.93812899822975	-1.63465299275476	1.50560200435147
H	6.97150998951653	-1.68439999346360	1.45248400136823
Ga	0.15346355208873	3.18018323476188	1.64218915401265
Ga	0.02884056272555	-2.26016545302610	1.58017198078155
Ga	-0.01743112894169	-7.55850048776990	1.41925888189724
Ga	0.06095537731836	8.71511043564044	1.41975747726135
Ga	-3.94560431897475	3.07542528214943	1.68862964104664
Ga	-4.01019028637887	-2.32769533218655	1.73114318551812
H	-3.10475300251846	-7.09476499655733	1.48839400198066
Ga	3.86930374418164	3.24927925724438	1.45304150333109

Ga	3.92791673220538	-2.24356113734535	1.56247057349810
H	3.09890599277410	-7.11695299868282	1.46470200392935
P	-1.89196350358172	4.34798379771377	-2.20804311651326
P	-1.93858309381771	-1.04754691948082	-2.18778126806717
P	-1.95420761298718	-6.48802471627176	-2.16192475110458
H	-1.27387694659519	9.36641798965587	-2.21995800617666
H	5.17135195865659	3.88265699050577	-2.24752408778136
P	5.78828901850820	-1.07994022346913	-2.19768576054209
P	-1.88854193231587	4.33725430092366	1.63165048971017
P	-1.98647181459921	-1.03144025502293	1.46143086414538
P	-1.96831933812035	-6.32339852200201	1.87677274503842
H	-1.24760878804920	9.57708500172875	1.66978798572177
H	5.18559706358507	4.10105302853161	1.63919001616902
P	5.85302643789633	-0.91667932590111	1.88481066489038
H	-0.02806298677979	-8.83358200627921	-3.50648998509638
H	0.03053900224743	7.47918004288458	-3.53721295903241
H	0.01098996769943	2.03992097734220	-3.52934496502334
H	-0.00859700607844	-3.40367200398577	-3.52729500055094
H	-3.84066699915588	2.04836798877097	-3.52197899917906
H	-3.86017099603494	-3.38591500195846	-3.50709999619206
H	3.86255302418325	2.02081902120535	-3.55139493203749
H	3.84304899708352	-3.41346500956809	-3.53651599787311
H	-5.12608800961839	3.91948400674943	-2.20820000077332
P	-5.78165040158997	-1.03630387602742	-2.14903019203183
P	1.95777117577755	4.36010675252036	-2.20480683460097
P	1.94860451629423	-1.06315604914372	-2.18807392008252
P	1.91440309688338	-6.51732043373590	-2.18966650296495
H	1.35847094445879	9.35700297940709	-2.23001102099953
H	-7.04391300921167	1.15820400235074	-0.25886000063085
H	7.08399498562979	1.10767898565898	-0.31281300150268
P	-0.01547830837453	-9.27715339554076	-0.25497979178483
P	0.05410281232086	7.13536226371245	-0.30673547443820
P	0.05568486002021	1.73479120501302	-0.24588546587273
P	0.00271388573253	-3.73799532161490	-0.29805329128676
H	-3.17969594573198	6.59650997907503	-0.27091400493080
P	-3.84788466888479	1.74936964723730	-0.27212940956080
P	-3.92272975984927	-3.73584077540822	-0.22205875199245
H	3.25904788416457	6.57348394363212	-0.29550204318446
P	3.82984020862699	1.67614973061730	-0.30893365048498
P	3.91393515939231	-3.77431454974973	-0.28431378315582
H	-5.10924899726937	4.13787100546401	1.67850299823411
P	-5.84202012315110	-0.85578644150420	1.97580616620692
P	1.98042839729433	4.56794865957377	1.89818635100749
P	1.97323330288035	-0.95569245712119	1.87895685953138
P	1.97209772675159	-6.32221477493422	1.83166726594367
H	1.36325776973574	9.56774795142986	1.65981697149499
O	-3.27903395795142	-3.38997737982334	3.18350205423645
O	-0.73459562191052	-3.39119760819930	3.14989497166960
H	-1.99120351167522	-0.22104733476597	2.60553796042839

H	-3.60782983633292	-3.10154892489299	4.04906334665833
H	-1.79353491849786	-3.40778436388712	3.18413697179840
H	-0.43369344088595	-4.30528824078927	3.27492210624294
H	-1.84853593198256	5.21757248504692	2.73730710548143
O	-4.00591552413703	1.89899252437113	3.16696918514292
H	-3.91613402008449	2.42017188774192	3.97982521121351
O	0.26433284199855	7.29820224814738	3.05885897774301
H	0.88726068675779	6.56786535867170	2.83425529326624
H	-0.57195697696652	6.85869825875359	3.28316286870959
O	4.04856982176759	1.71213123882020	3.01454282654967
H	3.41286528618864	0.97613785170037	2.88823739705978
H	4.92338272928349	1.27727451309631	3.03662579822215
O	3.65846363923633	-3.60957113213711	3.18501744667138
H	3.15625712265303	-4.42673183314276	2.97816940860229
H	4.46748041533916	-3.90063560131757	3.63799462002267
C	1.22220630980594	1.11937609675488	5.34579802815526
C	1.19203261645332	1.89497347547277	4.19406928417706
C	-1.08839034247089	1.55248580347856	3.93259842924069
C	-1.14042895819481	0.77758554076714	5.08588209585623
C	0.03570383455400	0.54155310943600	5.79962054101976
H	0.02589424030431	-0.06848010407202	6.69609653356963
H	-2.09178638408897	0.36826927196656	5.40650610567755
H	-1.99353298360982	1.75481338442607	3.36835143873035
H	2.07329413819465	2.40507710922263	3.83278837326751
H	2.15875695565259	0.97474326743796	5.87103638327644
N	0.06328401021755	2.09009637475019	3.48304626077310

Explicitly solvated surface without Py

Energy=-8724.51667517733

H	-1.93139900988870	5.16831499666156	-3.18721299278646
H	-1.92298199968140	-0.27851302939548	-3.20954199360141
H	-1.91455697216833	-5.72664397563700	-3.22984401687490
H	5.78024600374158	-0.26786100156534	-3.23053100272550
H	-1.11723898004941	-10.08642197758415	-0.11890500384862
Ga	-1.89238745946324	5.82812639835286	-0.10649232868189
Ga	-1.95952524884770	0.49345733410847	-0.15661628986621
Ga	-1.94014041833871	-5.04722142915910	0.01959618767705
Ga	5.75432087706753	0.39003032519154	0.03893113991763
H	5.01967798250675	-4.63295699722127	-0.11505499481107
H	-5.77458395811092	-0.28594797342366	-3.19590100850663
H	1.92021100745745	5.17434499775551	-3.19875599132210
H	1.92862800629415	-0.27248401927507	-3.22108500763477
H	1.93705298388981	-5.72061298926208	-3.24138801460982
H	-6.91759004371161	-1.88211603249351	-2.02920198546956
H	6.93519899292833	-1.86043299813723	-2.07071799964536
Ga	0.03233907766688	3.05925690005790	-2.13552304759270
Ga	0.01687228346175	-2.38485906378076	-2.13227252617067
Ga	0.00767793224317	-7.89286773465051	-2.11909301151260
Ga	-0.00650493738199	8.51448248924340	-2.09223747959079

Ga	-3.89324344074954	3.03521211690379	-2.09785784996839
Ga	-3.87991801808681	-2.44066507515719	-2.09573897351155
H	-3.05637702862787	-7.32226302865276	-2.06289098645784
Ga	3.88339977351453	3.03687542196315	-2.11810898396835
Ga	3.89545811851387	-2.41940337664681	-2.13304080752464
H	3.09082301323918	-7.31264201440206	-2.08131398628760
Ga	-5.73071407325928	0.35578382688901	0.06485543774714
H	-4.98173598667907	-4.64861299145506	-0.08508000949833
H	1.17200499052616	-10.08283800139259	-0.12576600133496
Ga	1.90571736528195	5.80814389338173	-0.02050258795106
Ga	1.95483687931703	0.32020219795982	0.00706423900154
Ga	1.97131389981762	-5.04094012059841	-0.03232349698607
H	-6.93525398448186	-1.64096097921808	1.68167299946035
H	6.97438498608511	-1.61918799280627	1.63998799910749
Ga	0.14457134824111	3.30512536244072	1.54020794633362
Ga	0.03061729179482	-2.21838917992417	1.76748456769859
Ga	0.01695932342108	-7.53102645480725	1.58075560163714
Ga	0.00911416887906	8.74935296359079	1.65290201415932
Ga	-3.96281396267370	3.07402816094576	1.93767974630909
Ga	-3.98363004721450	-2.32083612082481	1.90386870166726
H	-3.07384500754819	-7.08113600676672	1.64835800176587
Ga	3.84890619444786	3.28911082534518	1.67569061491140
Ga	3.93877858664698	-2.19269365909225	1.76117121108361
H	3.12981400590987	-7.07142600689989	1.62976499780482
P	-1.92033650659849	4.38081803278433	-2.00869820300744
P	-1.93943253261518	-1.02336852164845	-2.00971522815559
P	-1.92198809624453	-6.45757163006221	-2.00066050912941
H	-1.32479398391660	9.40197299906904	-2.00017100054049
H	5.14853899981331	3.95158000509527	-2.04174799941106
P	5.79207923479578	-1.00707540237343	-2.00854887187200
P	-1.91088065664732	4.34354726199928	1.83768092549658
P	-1.98194690762064	-0.96645336434910	1.68693745443979
P	-1.94050930081486	-6.30693636078996	2.03880515957689
H	-1.30268599402207	9.59892500304475	1.89024500291383
H	5.15858899574441	4.15620999853844	1.84565399526510
P	5.85408685824861	-0.85388369195203	2.07901472901553
H	0.01567499980986	-8.78633200170304	-3.34998199303470
H	-0.00965300442019	7.52618600151300	-3.32297599811020
H	-0.00121500284325	2.08701599798512	-3.33435799959773
H	0.00721200071699	-3.35646597476891	-3.35157100484074
H	-3.85283800884931	2.07568601977080	-3.33017698114796
H	-3.84438701054923	-3.35853298332362	-3.33452799585194
H	3.85038199968623	2.08774499974557	-3.35326099999708
H	3.85883299962113	-3.34647398612082	-3.35761300116375
H	-5.14889998252159	3.93545998596811	-2.01088701362258
P	-5.77589908396683	-1.02869839082064	-1.97669311598925
P	1.93742928650867	4.41372132105564	-1.99956013619127
P	1.95783993755108	-1.02187680232517	-2.00928308590815
P	1.94596147803723	-6.46244152946787	-2.02208471562346

H	1.30755399157302	9.40609299882260	-2.00806000078058
H	-7.05401399619172	1.15752096884818	-0.07295800416279
H	7.07389399982361	1.17963699766801	-0.11530000021377
P	0.02810055638730	-9.24180438561060	-0.10026497140716
P	0.00777729515711	7.17597190098035	-0.08560131218732
P	0.04538218903892	1.70540144575170	-0.13473440354608
P	0.01225660176023	-3.69407030838341	-0.11710421481910
H	-3.21785799024516	6.61546799717127	-0.06255900583858
P	-3.86428192933700	1.78781651972461	-0.07397617991971
P	-3.90178633765884	-3.72324669247349	-0.05270349196686
H	3.22088599026162	6.62554799857427	-0.08185499974311
P	3.82350170319930	1.73534196472257	-0.10536519656838
P	3.92999105662787	-3.71514959926481	-0.09987546386407
H	-5.13625699696029	4.14009500151942	1.87650699793948
P	-5.82337299092520	-0.86070435696182	2.11550098515972
P	1.93672387768492	4.58800395774549	2.12468783071887
P	1.96986923659895	-0.91087078832794	2.06972854162759
P	1.99868280207482	-6.28422333659293	1.99944557679266
H	1.30818198860898	9.60301299661744	1.88242099927894
O	-3.27625905769862	-3.39665102158940	3.35087601806507
O	-0.72567962284777	-3.38282506807576	3.31452872072390
H	-2.00043146951574	-0.10442423240654	2.80277177851428
H	-3.57986501056318	-3.07515006805779	4.21457942938769
H	-1.78246451241326	-3.40766454453001	3.35023052340888
H	-0.41912412088725	-4.29666645447648	3.42682286892885
H	-1.72143815188356	5.22043052582948	2.92562845777947
O	-3.88188067034075	1.97203488995964	3.46363808123126
H	-4.41244306260981	1.17252160923736	3.32267316298945
O	0.23020687055990	7.37509628634980	3.30886243953833
H	0.80701469830975	6.61071883837499	3.08567942973321
H	-0.59749280313438	6.99064203642000	3.63930582228350
O	3.94552683316669	1.82749759783247	3.27391069200774
H	3.22202335383975	1.16946703016326	3.21894695055453
H	4.76508860711259	1.29520276014635	3.26429904024047
O	3.66621576264220	-3.56732116707832	3.37012531785834
H	3.17780650997974	-4.39066407201656	3.15466930034556
H	4.47235069827119	-3.84832991339368	3.83462346726609

7) HCOO⁻

HCOO⁻ on explicitly solvated surface

Energy=-8837.36156839686

H	-1.94553298931725	5.18264000617566	-3.22600401227449
H	-1.91849201369159	-0.26399395381395	-3.27763801088704
H	-1.89143499532371	-5.71193998919751	-3.32725000161611
H	5.78474392194807	-0.22693194647570	-3.31074601055622
H	-1.07425492345092	-10.08572899110376	-0.24104600088689

Ga	-1.86605407436117	5.90488806786885	-0.22610141856623
Ga	-1.89441030741045	0.44597838390464	-0.12498278035996
Ga	-1.89995868803314	-5.04677860927646	-0.07061197626396
Ga	5.74974344478808	0.42276953359687	-0.03751711915649
H	5.04404700684953	-4.61138202157207	-0.21756901959485
H	-5.77008499720955	-0.28464897507983	-3.25794799763353
H	1.90607699148770	5.20187899144651	-3.24360300958740
H	1.93311799623987	-0.24475398135110	-3.29523602541103
H	1.96017491871142	-5.69269991969269	-3.34485103296301
H	-6.90579002260337	-1.89099501320623	-2.09803600536448
H	6.94699906323143	-1.82180006200468	-2.16133298186850
Ga	0.03429258019186	3.05448104795031	-2.15601677571609
Ga	0.01407382253556	-2.37158223975493	-2.20661690074357
Ga	0.04209212870071	-7.87260795967919	-2.23208254548991
Ga	-0.02290649879278	8.53926725905592	-2.12755001055597
Ga	-3.88841281085624	3.03718387626260	-2.14329247679501
Ga	-3.84672682840814	-2.43192597954893	-2.17033276882918
H	-3.02595600932407	-7.31773400489507	-2.16708400133017
Ga	3.86987242511598	3.06258057840116	-2.16574271032132
Ga	3.88697129219174	-2.38059722001947	-2.22209390021783
H	3.12124410421608	-7.28703009150931	-2.19517297628079
Ga	-5.72214949376141	0.34455444422000	0.05368501157836
H	-4.95736601829815	-4.66133901239824	-0.17186899878003
H	1.21498892636424	-10.07429398549068	-0.25150601131314
Ga	1.89765022233335	5.76730966615487	-0.01190661509021
Ga	1.90988677158314	0.36761863442704	-0.04682336709202
Ga	1.98108559353502	-5.01371377400010	-0.11589745255080
H	-6.91841308763833	-1.66990503249558	1.61413099309573
H	6.99122596126909	-1.60042597991417	1.55057501135286
Ga	0.05077983948733	3.09027755717286	1.83052782490347
Ga	-0.12491888957911	-2.14987654624511	1.65239841805472
Ga	0.05932430695331	-7.53286424649988	1.47889962675842
Ga	-0.00680920990803	8.74254498306275	1.60877990293009
Ga	-3.83076843476824	3.24562639710268	1.64426357214776
Ga	-3.76601418270517	-2.17785756554266	1.71118705731936
H	-3.03838299885654	-7.09667298885855	1.54545699582029
Ga	3.82682601493814	3.30209602518579	1.63576506507402
Ga	3.91707696737344	-2.16851510029871	1.65529842606152
H	3.16527698481675	-7.06568699827531	1.51711000102720
P	-1.91963145569544	4.39205390507182	-2.05920162347268
P	-1.92923932211028	-0.99855730744196	-2.06575724472534
P	-1.89371385752247	-6.45041041304170	-2.10112367442500
H	-1.35154801750999	9.41193401995022	-2.01716399135955
H	5.14045700581616	3.98390901091894	-2.09828398085398
P	5.79687913935069	-0.97429118694301	-2.09241041473196
P	-1.85057963213812	4.49789713368369	1.67061044812222
P	-1.93968646714382	-0.72807635458596	1.86939203585156
P	-1.90502965711389	-6.33485298557306	1.93772618760654
H	-1.32396300425044	9.58798999823356	1.87424100083295

H	5.15595199815378	4.16761699925507	1.79016700118087
P	5.85694776885809	-0.84976963067183	1.98723382568416
H	0.04910799688619	-8.76436600923482	-3.46689198030351
H	-0.03205901043420	7.54778296506124	-3.35212503224572
H	-0.00500599348000	2.10874903424252	-3.39276898155290
H	0.02204200278468	-3.33456702284954	-3.43926900187203
H	-3.85662298747479	2.08424896409899	-3.38256003222733
H	-3.82956199359612	-3.34987199204676	-3.41614794936088
H	3.84659699487008	2.12272698686857	-3.41775702178161
H	3.87365801357483	-3.31139400886960	-3.45134598363286
H	-5.15698203717723	3.93247103527933	-2.05123199316993
P	-5.76451776003317	-1.03073726658013	-2.03439520568696
P	1.92478300746555	4.43661991344262	-2.04537005292804
P	1.95128908778234	-0.98704476740386	-2.07726601152765
P	1.97524676031207	-6.43587236630972	-2.12367192283056
H	1.28080102042666	9.42508202606498	-2.02919298335906
H	-7.04953590164420	1.13760697363998	-0.12524898292670
H	7.07837205915552	1.20817701050801	-0.18980401399115
P	0.06881137788885	-9.23555592838335	-0.21841704181945
P	0.03911415293158	7.21063175217549	-0.15213050348643
P	0.02813746747073	1.78352878095746	-0.15156500092115
P	0.02575942978294	-3.68045660665235	-0.19835995624498
H	-3.23202099070233	6.60854599365762	-0.09156199974286
P	-3.83408167512211	1.74273660246421	-0.15471053572487
P	-3.86527489948620	-3.73785579164618	-0.14125089497084
H	3.20672298224981	6.64070899161197	-0.12098200097052
P	3.81528365786766	1.75337681102088	-0.16194977041445
P	3.94734673755215	-3.69824112730716	-0.20225396275764
H	-5.13889498200132	4.11619398959615	1.83720699335296
P	-5.78044937218999	-0.93213824188230	2.07212133390862
P	1.88525917911782	4.53602544633413	2.08812594184687
P	1.93013561309193	-0.93547884900200	1.97507278360629
P	2.03621082257122	-6.28695952401448	1.90414898068897
H	1.28690499954903	9.60103199870638	1.86231200238478
O	-0.58489568396313	2.01447863763915	3.31706273053611
H	-2.22050237345506	2.03208916929145	3.31778106993655
H	-0.40276650008726	1.07011865815640	3.17720018529029
H	-1.93371253087109	5.33582283032192	2.80419412869473
O	-3.24205483924228	2.10852294880472	3.30174440511307
H	-3.49910874468526	2.50971394500179	4.14754373036901
O	0.22214229719709	7.30559277592584	3.22098636368487
H	0.82510935454309	6.56130482046757	2.98143090315609
H	-0.61324879834587	6.88182606459401	3.47533046195379
O	3.91297842688852	1.76330881116467	3.19258999170621
H	3.21897934457689	1.08254231350740	3.04814446024719
H	4.74961095732989	1.25826067865082	3.18464050421499
O	3.70509834207983	-3.59612721095145	3.24606709631926
H	3.13429295908794	-4.37257822971410	3.05856716884714
H	4.52604093793584	-3.94905509926493	3.62670845930170

O	-3.04189319784854	-3.40676870106899	3.25080362888521
O	-0.73604268895587	-3.42742535378591	3.18550353463681
C	-1.87953683451173	-3.69540310389051	3.67850327280924
H	-1.85712853068261	-4.26174851727032	4.61954955249563

Explicitly solvated surface without HCOO⁻

Energy=-8648.08846141317

H	-1.94553297533519	5.18264000051009	-3.22600401124295
H	-1.91849193710830	-0.26399390704179	-3.27763811026928
H	-1.89143500081583	-5.71193999046725	-3.32725002240112
H	5.78474392546718	-0.22693195955026	-3.31074600931200
H	-1.07425493974890	-10.08572899797887	-0.24104599314299
Ga	-1.86657554899014	5.90516114037375	-0.21576804359602
Ga	-1.88837475805268	0.39916560427308	-0.04809832514207
Ga	-1.89829008512941	-5.06911800119687	-0.08161760872483
Ga	5.75686124395464	0.42195643331570	-0.04058411670536
H	5.04404702215501	-4.61138201859401	-0.21756901431657
H	-5.77008496076180	-0.28464898236090	-3.25794796717547
H	1.90607700421957	5.20187899121953	-3.24360301004159
H	1.93311796799482	-0.24475400114259	-3.29523602141184
H	1.96017491813594	-5.69269992107934	-3.34485103974124
H	-6.90579004763171	-1.89099502832101	-2.09803603942876
H	6.94699906256681	-1.82180006106908	-2.16133298033050
Ga	0.01821711263526	3.05014524826588	-2.15474009166840
Ga	0.02336781571893	-2.35436213902237	-2.23412795980024
Ga	0.04562422688359	-7.88649801362397	-2.22454194238773
Ga	-0.02334687273469	8.53985785453585	-2.12811912750748
Ga	-3.88295660744235	3.03406025288262	-2.14119626922096
Ga	-3.84848905365778	-2.41473692522481	-2.19811426797875
H	-3.02595600921507	-7.31773400355351	-2.16708399602695
Ga	3.86984021751671	3.07775696330597	-2.18161583172483
Ga	3.90204807490148	-2.37883853261223	-2.23030762212142
H	3.12124410970061	-7.28703009682800	-2.19517297380720
Ga	-5.72716571511343	0.37297084731208	0.01147503872934
H	-4.95736607368182	-4.66133910090689	-0.17186901842704
H	1.21498893981571	-10.07429398466171	-0.25150600744162
Ga	1.89664293847600	5.77025411253183	-0.01116201712888
Ga	1.95366963389508	0.42274684659684	-0.09872771597042
Ga	2.02111264902059	-5.04761627067583	-0.13302944492712
H	-6.91841305410522	-1.66990502024412	1.61413099373141
H	6.99122598163149	-1.60042599324213	1.55057500964657
Ga	0.04908132516944	3.08913042305831	1.83810117045903
Ga	0.04975776078600	-2.07203867791422	1.41973023816148
Ga	0.05585401558355	-7.51902496106096	1.49743093063039
Ga	-0.00716336147740	8.74458797593261	1.61270448973101
Ga	-3.83479243968239	3.23655920303887	1.67599441278074
Ga	-3.91022719286410	-2.09604545805730	1.51563528831290
H	-3.03838298276941	-7.09667297240852	1.54545699732322
Ga	3.82721229465431	3.31612004879669	1.64605771351706

Ga	3.95540582853177	-2.16977365530213	1.63811966927996
H	3.16527697817365	-7.06568699407667	1.51711000453561
P	-1.92290201734825	4.39623105309009	-2.05473646477395
P	-1.92640458675540	-0.99592521202210	-2.05502154328425
P	-1.89031013377361	-6.45760330230761	-2.10719394218419
H	-1.35154802184123	9.41193402524151	-2.01716398876416
H	5.14045698984849	3.98390898982689	-2.09828400079143
P	5.80119100429869	-0.97082041174428	-2.09239700122954
P	-1.85453125969391	4.48773071210129	1.68111438827013
P	-1.91344863816882	-0.95489121561472	1.97575907493008
P	-1.92133014760645	-6.30146142368004	1.94891981778265
H	-1.32396300328548	9.58799000041317	1.87424100217406
H	5.15595199047146	4.16761699396472	1.79016699782972
P	5.86777712574603	-0.83933754401596	1.98966181090234
H	0.04910799862632	-8.76436601909828	-3.46689200016107
H	-0.03205901164574	7.54778295777772	-3.35212503669902
H	-0.00500600562208	2.10874902099313	-3.39276900520132
H	0.02204198822020	-3.33456696037127	-3.43926889858103
H	-3.85662300478394	2.08424896207865	-3.38256006157972
H	-3.82956201845588	-3.34987195593742	-3.41614788104867
H	3.84659699944894	2.12272701549142	-3.41775699445642
H	3.87365801499083	-3.31139400101499	-3.45134601076756
H	-5.15698201070130	3.93247101408643	-2.05123197933992
P	-5.76742766059531	-1.02990951518789	-2.03873175377051
P	1.91654916625036	4.43354279085693	-2.04340708389168
P	1.96300181021185	-0.98336281226590	-2.08053687263355
P	1.97500540059491	-6.44488695648500	-2.13118385969560
H	1.28080102685590	9.42508203184978	-2.02919298183991
H	-7.04953595006519	1.13760698611527	-0.12524896978467
H	7.07837205996491	1.20817702564892	-0.18980400919838
P	0.06720711033118	-9.23333053907487	-0.20517084198935
P	0.03776341933389	7.21005423098774	-0.14787423559328
P	0.01984707504364	1.76136086973752	-0.13430659750611
P	0.05389287526562	-3.73403924915324	-0.24721609855146
H	-3.23202099624075	6.60854600254866	-0.09156199492730
P	-3.81094451658932	1.72548145776748	-0.12840866064064
P	-3.86377975627822	-3.75728040429542	-0.17598043308769
H	3.20672297129838	6.64070898536229	-0.12098200032556
P	3.84398386072644	1.78508906708913	-0.16851373347503
P	3.95425512715775	-3.69550298717898	-0.21098139886046
H	-5.13889497038183	4.11619398084495	1.83720699182047
P	-5.82270897160523	-0.87724597272920	2.06533751085524
P	1.87966425490384	4.53463893944942	2.09151459244201
P	1.99228500731378	-0.87911576711948	1.93231728658489
P	2.04270035909985	-6.27797943312653	1.90368181443205
H	1.28690499922724	9.60103200095603	1.86231200427155
O	-0.61738847623270	1.98719255322822	3.29353798925356
H	-2.21655044178098	1.97205273276468	3.29975751755829
H	-0.35285206495643	1.05685749364643	3.21033740298139

H	-1.92189072317165	5.32261243894010	2.81677894188844
O	-3.24360249780398	2.01865440425624	3.26192559366509
H	-3.54958315609068	2.30753079389817	4.13614430546981
O	0.21536475400431	7.31606066343189	3.23049231843350
H	0.81054762326919	6.56496717908375	2.99653699197321
H	-0.62179627448650	6.90442025810554	3.49820234455025
O	3.95833336373343	1.80971688823328	3.21765584876862
H	3.24968946746841	1.13890233749811	3.13442003252028
H	4.78737344238822	1.29286571464528	3.19732452138603
O	3.70151674219237	-3.55082875006988	3.24501626883833
H	3.12604694809427	-4.32716662125259	3.07505651873435
H	4.51276699470939	-3.89596724918981	3.65309252456584

8) OH⁻

OH⁻ on explicitly solvated surface

Energy=-8800.47843462172

H	5.77741515587200	18.48719916910554	2.80454894857052
H	5.77741493342276	13.04046339292196	2.76833021407921
H	5.77741492969626	7.59242008537318	2.73413664055220
H	13.48063509373573	13.03905259545778	2.77042344180210
H	6.55859741612217	3.22350854989928	5.83627544776833
Ga	5.82183752360018	19.14316609110817	5.95480155924281
Ga	5.75869485469061	13.85161950947814	5.81657799558208
Ga	5.73807733181016	8.27086848738335	5.98592415386506
Ga	13.43591157576573	13.69766079369376	6.03670034253072
H	12.70392631545764	8.66726174040577	5.87242507777015
H	1.92580495883615	13.03905183054179	2.77042457427244
H	9.62902519508823	18.48719931797471	2.80454880724616
H	9.62902505323257	13.04046305701634	2.76833078452074
H	9.62902482235952	7.59242103476708	2.73413538974358
H	0.77682474615581	11.44172602621216	3.92960753842394
H	14.62961388852700	11.44172602477429	3.92960798770790
Ga	7.71882795292357	16.37091000851938	3.87587736442204
Ga	7.70549217815850	10.94169538772874	3.83928250282831
Ga	7.69138505680925	5.42255101596162	3.84452897841704
Ga	7.70806893571463	21.82424331962852	3.91641774147696
Ga	3.82946439337069	16.36091611392249	3.88991219794209
Ga	3.81027715074866	10.89391353935969	3.86625914787904
H	4.62962023890229	5.99564053322508	3.89357731123667
Ga	11.56906293581233	16.35110547881452	3.89106414622667
Ga	11.57198135577750	10.89867850983656	3.85660325531504
H	10.77682056294447	5.99563917629857	3.89357707360083
Ga	1.98650164071174	13.71718289631458	6.08667544269034
H	2.70251348724950	8.66726136468111	5.87242540945626
H	8.84784132465705	3.22350893137773	5.83627572910780
Ga	9.59800283120576	19.08833198794580	6.03987194281079
Ga	9.58981804467556	13.69508571345849	6.00906468397573
Ga	9.65688668735430	8.26469652873722	5.94222873818672

H	0.74840065479676	11.67346249490079	7.64098897185884
H	14.65803972663314	11.67346263157694	7.64098961248448
Ga	7.60354841622725	16.62538545885982	7.74784333732982
Ga	7.70499707545529	11.07435282820639	7.71954503286097
Ga	7.69086319196810	5.77652980705574	7.54360598544329
Ga	7.70420083823200	22.03355130697964	7.64271032548685
Ga	3.96305540037352	16.62392561818782	7.82281832812740
Ga	3.68833626699484	10.99419681201071	7.86327974934909
H	4.60139082875629	6.22734720768093	7.60533347689435
Ga	11.51097982201691	16.60307609970369	7.68369179854576
Ga	11.60287924036621	11.12575858380820	7.74561633124930
H	10.80504968595534	6.22734636996115	7.60533299614117
P	5.78642401840110	17.72197673270049	3.99807444301001
P	5.75320094425663	12.30491053343566	3.97295925335251
P	5.76366152477679	6.86002239758594	3.96285443219987
H	6.38704550767642	22.71684346405709	4.00420321839050
H	12.85194059083947	17.25642353146722	3.96807753544931
P	13.48511741768115	12.29546248416406	3.99029381286249
P	5.80816246728683	18.06375574076158	8.04103872913013
P	5.69539746245628	12.31526652039444	7.61351061941592
P	5.73373342797557	7.00044287226455	8.00080419661272
H	6.39778624020222	22.90385782680830	7.89512872470398
H	12.85064306397999	17.45114201454195	7.85597218469060
P	13.53533728402584	12.44181833156069	8.07349170272777
H	7.70321980427650	4.53002828093239	2.61196078706584
H	7.70322008006753	20.84237176453965	2.68056193730804
H	7.70322004814795	15.40326644775434	2.65531094161418
H	7.70321993853525	9.95986304434736	2.62421704304926
H	3.85161002586030	15.39798404453488	2.64793621237590
H	3.85160997437805	9.96381134244492	2.62972792254314
H	11.55483006852358	15.39798442637466	2.64793744110709
H	11.55482989273544	9.96381196445446	2.62972870796164
H	2.55450154925575	17.25642173740177	3.96807763417670
P	1.91442141133012	12.30957258059552	4.00262212063851
P	9.63129708657369	17.73032052502523	4.00929659338977
P	9.64192741268922	12.31073743998826	3.99346425461712
P	9.63348720769686	6.84687622046755	3.95135419181075
H	9.01939441919883	22.71684271740827	4.00420261910024
H	0.63926641797549	14.47657188324411	5.89317725857022
H	14.76717408431327	14.47657318865466	5.89317634366648
P	7.70510875205928	4.06675755283134	5.86016195242707
P	7.72584093559016	20.50009765290928	5.88342637909925
P	7.71245319301134	15.11362881758383	5.90430125313048
P	7.70041866663688	9.60482043444233	5.84232184953623
H	4.48384883067006	19.92840936948946	5.92900072827962
P	3.85274018606343	15.14317277501593	5.92438250983040
P	3.77784076986209	9.59510388414973	5.90536774731603
H	10.92259265572404	19.92841059124193	5.92900143825008
P	11.51307412616420	15.04019513786099	5.90049113871166

P	11.61462299365023	9.59029585551307	5.88639056179622
H	2.55579672854080	17.45114106314538	7.85597167043343
P	1.84850125016896	12.45079048007378	8.11105635122572
P	9.58415062388785	17.83890277496232	8.13363122633621
P	9.62488810484918	12.40267398605216	8.05316866342358
P	9.67415900375744	7.01623681523053	7.97221777621466
H	9.00865268855616	22.90385817515298	7.89512902843331
O	4.39383641280625	9.90352637219603	9.30642177910565
O	6.94106860662279	9.92566778505411	9.28129357817431
H	5.64941185094788	13.11918817192747	8.76652944884277
H	4.09762678100635	10.24108089848583	10.16665493865081
H	5.88184200497948	9.89463385868685	9.30788105452143
H	7.25420367197840	9.01676408575128	9.41264359872358
O	4.44851495580677	15.27522946296268	9.21013145837355
O	6.96730893053075	15.28318998116633	9.23823953702584
H	4.15722692466654	15.56192946673136	10.08972464710233
H	5.89423407661153	15.24583459398791	9.24934532441946
H	7.32187774363331	14.38147447116534	9.20175996321798
O	7.71359612340303	20.53835749424552	9.23108835843911
H	8.50120650190881	19.95981946142109	9.12641090669434
H	6.96850337323999	19.90811487682499	9.05928014341928
O	11.65014709587313	15.10995052623775	9.28403904789499
H	10.93348635168977	14.44657222847333	9.21649397979994
H	12.47285645664624	14.58364985460287	9.25200548690568
O	11.32379368479974	9.74372626347683	9.35404545347098
H	10.83969881678907	8.91980287686790	9.13196103425215
H	12.13043109754552	9.46236626303701	9.81729648292617

Explicitly solvated surface without OH⁻

Energy=-8724.51835394603

H	5.77741509427652	18.48719922990869	2.80454894753945
H	5.77741495744660	13.04046333622717	2.76833019018033
H	5.77741493616097	7.59242008865883	2.73413663898301
H	13.48063510419763	13.03905258547735	2.77042344156505
H	6.55859740621290	3.22350856613287	5.83627545368387
Ga	5.80430877365203	19.11221564376431	5.99576453238027
Ga	5.76242130135580	13.81270906923785	5.81359630316465
Ga	5.74635233156782	8.26078602707978	5.98352086660165
Ga	13.44353294385264	13.69079557596903	6.03952040660171
H	12.70392631019775	8.66726174062378	5.87242508630418
H	1.92580499254922	13.03905180493390	2.77042460616412
H	9.62902517248743	18.48719932974919	2.80454878131086
H	9.62902505826434	13.04046303013516	2.76833077601329
H	9.62902485362260	7.59242100387164	2.73413540105478
H	0.77682471868435	11.44172601200119	3.92960751585499
H	14.62961387638646	11.44172603073606	3.92960798824610
Ga	7.72252315673958	16.37385766598362	3.86429567181879
Ga	7.71665539151963	10.93105776104599	3.84337752794434
Ga	7.69374268707760	5.42021655119001	3.84498367419471

Ga	7.70317983048463	21.82237277059457	3.91897586295774
Ga	3.82772633711817	16.37366485691164	3.86213286068311
Ga	3.81912684536599	10.87904454971767	3.87058034561606
H	4.62962022508668	5.99564052470620	3.89357731162202
Ga	11.57805065757353	16.34825826759843	3.88596440374507
Ga	11.58291863303364	10.89297955147589	3.85612561761211
H	10.77682052131859	5.99563921324513	3.89357706307153
Ga	1.96031921698033	13.67347320928026	6.02629332005023
H	2.70251349327416	8.66726136844242	5.87242540195940
H	8.84784134585994	3.22350891524500	5.83627572903401
Ga	9.60131727207333	19.11405369951189	5.99871450688946
Ga	9.63198541658221	13.65385761861072	6.01046151594227
Ga	9.65697026538201	8.26278150852159	5.94352734893539
H	0.74840067275238	11.67346249792256	7.64098896635137
H	14.65803972987685	11.67346262896051	7.64098960775426
Ga	7.70233984555150	16.69339945225484	7.55691877637288
Ga	7.72187187006469	11.07921068347998	7.73642984751222
Ga	7.69253757653747	5.77198034279123	7.54574347791761
Ga	7.70320087258168	22.04028451080864	7.65742522709513
Ga	3.88173129737928	16.60518575150420	7.66950145946673
Ga	3.71581595569024	10.98096119241999	7.86583216306253
H	4.60139081738116	6.22734720569193	7.60533347767893
Ga	11.52291981670525	16.59949570114948	7.66993379661450
Ga	11.62038373024260	11.10818946454192	7.74696740790935
H	10.80504969618051	6.22734637018812	7.60533299625419
P	5.78716251396454	17.71989579578564	4.00305883804710
P	5.76028109767420	12.29132385888414	3.96490800116217
P	5.76572119151388	6.85724147404806	3.96067051241925
H	6.38704553290126	22.71684348407181	4.00420322165191
H	12.85194059509064	17.25642351049445	3.96807752694137
P	13.48716150552317	12.29625276045737	3.99037766831234
P	5.79740371374537	17.87277320711167	8.11285461967903
P	5.71361831934402	12.33375360405528	7.64835987952344
P	5.73549985128473	6.99794738678360	8.00074440183513
H	6.39778616474622	22.90385785542998	7.89512872556827
H	12.85064300180310	17.45114202146224	7.85597217267490
P	13.53782149581627	12.44017472705988	8.07717627247484
H	7.70321980988540	4.53002829163174	2.61196078784334
H	7.70322007312642	20.84237175161232	2.68056191770411
H	7.70322006196698	15.40326647706909	2.65531098328342
H	7.70321993535881	9.95986308115413	2.62421704583046
H	3.85161009658386	15.39798393919610	2.64793618834485
H	3.85160995565364	9.96381138466065	2.62972792487013
H	11.55483007745542	15.39798445148732	2.64793745889106
H	11.55482988730103	9.96381198499807	2.62972870257324
H	2.55450144087686	17.25642183411033	3.96807764797845
P	1.92170092559473	12.29122116930284	3.98596824130888
P	9.63549126984613	17.72669328302523	4.00469665086297
P	9.65036529899993	12.30055736461312	3.98678997427432

P	9.63345473275968	6.84701162526974	3.95129458464960
H	9.01939439279277	22.71684270630617	4.00420262137407
H	0.63926643694605	14.47657187614879	5.89317726655879
H	14.76717407711475	14.47657318890343	5.89317634805656
P	7.70527433327324	4.06608133781125	5.86045463643184
P	7.70250319815907	20.48356917855119	5.90923081345219
P	7.73227149349357	15.05253946492595	5.88455444595018
P	7.70076073542961	9.60918493653340	5.85148272713680
H	4.48384904972427	19.92840923510868	5.92900072812351
P	3.83996109705274	15.08621218059234	5.86483504510144
P	3.78688174354564	9.58773139333963	5.90809940294829
H	10.92259264870729	19.92841060104598	5.92900143374434
P	11.52039111864889	15.03865038960499	5.89346059359416
P	11.61584032679894	9.58725891261139	5.88488202993959
H	2.55579665646578	17.45114109856848	7.85597167631654
P	1.87304899678527	12.43808981185245	8.06763455895582
P	9.60798989026457	17.87503128186870	8.11237896997063
P	9.65328604383502	12.38828250225016	8.05719917811818
P	9.67406396814714	7.01538381074740	7.97308108659135
H	9.00865276172375	22.90385817170586	7.89512904616041
O	4.40625380344748	9.90363431312850	9.31613087686231
O	6.96167247704513	9.91366534426236	9.28469169897420
H	5.70803769930337	13.17845794814778	8.77587759804550
H	4.10062007433184	10.22894844612783	10.17766176254253
H	5.90765485647405	9.88936069964551	9.31884688780113
H	7.26745528813606	8.99952652757379	9.39643306874791
O	3.73326048745706	15.07325658580428	9.18375010321687
H	2.95893829532582	14.48433858310535	9.08232132795936
H	3.70246924008373	15.39453938417505	10.09948770020067
O	7.70308361947631	20.56915851382937	9.27217735521821
H	8.47152765287753	19.96728395328307	9.16623124826727
H	6.93568966709444	19.96642875078642	9.16443632735503
O	11.63060835425693	15.12816678063372	9.27415148177526
H	10.90326982829178	14.47510869708467	9.21860702739158
H	12.44649524821159	14.59104915105169	9.25239578377268
O	11.34423546506841	9.72684295526293	9.35299994355382
H	10.85100384974590	8.90724610443703	9.13501461042296
H	12.15077949587493	9.43892246007656	9.81247036888057

9) $\text{H}_2\text{O} + \text{H}^+$

$\text{H}_2\text{O} + \text{H}^+$ on explicitly solvated surface

Energy=-8724.97494863362

H	-1.97421400318463	5.19229800744303	-3.18856200145468
H	-1.96548399953013	-0.25441999397191	-3.22725200325830
H	-1.95675600356804	-5.70244700127159	-3.26391599503121
H	5.73773199604467	-0.24361597815867	-3.20565201979390
H	-1.17650000125197	-10.07152700044784	-0.16178099781101
Ga	-1.91738974543950	5.88756896171481	-0.13212827100913

Ga	-1.94152540159007	0.48653600446484	-0.18232214894607
Ga	-2.00439261717683	-5.04238765246368	-0.01497235692930
Ga	5.69429749138128	0.40759224793829	0.06734992206643
H	4.96010300737228	-4.61804500559569	-0.10759999868102
H	-5.81709698871475	-0.26193998279694	-3.23491101215341
H	1.87739498308462	5.19840598449974	-3.17881001234990
H	1.88612498887618	-0.24831200154468	-3.21749801235694
H	1.89485399371224	-5.69633699564094	-3.25416400087643
H	-6.96647801286032	-1.86161401808194	-2.07936199038979
H	6.88630900757791	-1.83964700827636	-2.04428198938946
Ga	0.00120125607773	3.08692554441984	-2.13842678733199
Ga	-0.02636530609387	-2.36898387403100	-2.14905604463699
Ga	-0.03999303427440	-7.87432659816469	-2.14769730210255
Ga	-0.05312372048472	8.54324308532135	-2.08280424376333
Ga	-3.93070820747465	3.08256568872914	-2.16000544370770
Ga	-3.93015901440253	-2.42825208068694	-2.12655761632723
H	-3.10495299600397	-7.30157199709822	-2.10810700048016
Ga	3.83639870589322	3.05817894193316	-2.09482631841089
Ga	3.85773673119135	-2.40162278770434	-2.12488485718962
H	3.04224600359766	-7.29182500569947	-2.09253999426952
Ga	-5.82966046920373	0.32779167632804	0.04465537588692
H	-5.04130900365607	-4.63390599992079	-0.13292600108199
H	1.11274400055530	-10.06789599612398	-0.15598299925173
Ga	1.85248169369383	5.79944467303707	0.02544167287784
Ga	1.89039077062525	0.34035046387368	-0.02912708527603
Ga	1.91809419994669	-5.03446211280919	-0.04417714841802
H	-7.00466599974136	-1.63160700626866	1.63205300217571
H	6.90496900518191	-1.60954899342370	1.66727700725568
Ga	0.14797523560201	3.13399085224087	1.73441613812687
Ga	-0.04835400937359	-2.24052804969282	1.72915586492682
Ga	-0.05109048218154	-7.52188139825837	1.55333875519664
Ga	-0.05981557554801	8.76242736444720	1.67713357679378
Ga	-3.95201799087282	3.34789747713889	1.44953732953731
Ga	-4.06116544938832	-2.31598900694697	1.88414027237639
H	-3.14294900332205	-7.07159500147530	1.60368400188604
Ga	3.77751244458926	3.30029139876918	1.71151064972743
Ga	3.89354787102868	-2.18225563995199	1.78141676841285
H	3.06070900381673	-7.06175799779580	1.61939199898795
P	-1.95521386710777	4.40644629049022	-2.01147189442025
P	-1.98431422802173	-1.01273266994444	-2.03673457811797
P	-1.97081959891658	-6.43901380425895	-2.03850045493227
H	-1.37432998987788	9.42236299232590	-1.98544599840359
H	5.09931495609873	3.97221398218899	-2.00767698705530
P	5.74537443924845	-0.98414255763364	-1.98450789844006
P	-1.89174171934752	4.34409973135307	1.81455153623282
P	-2.04171600036382	-0.96712080717984	1.65995629570219
P	-2.01213154233854	-6.29884173316434	2.00412463088968
H	-1.37373801661823	9.60762899274924	1.90559299571948
H	5.08786502909536	4.16516506743890	1.88030306500243

P	5.79308885323542	-0.83397851375764	2.11099897277272
H	-0.02578500043450	-8.76172800048965	-3.38260399986950
H	-0.05183099972425	7.55058000820102	-3.30660498574549
H	-0.04313999862047	2.11148800609252	-3.33432300084488
H	-0.03442899902180	-3.33190000305123	-3.36788600150977
H	-3.89472200313921	2.10010200118781	-3.35145299523279
H	-3.88605699902456	-3.33406200088134	-3.37212599874782
H	3.80849602709464	2.11231699211565	-3.33194504703569
H	3.81716100532795	-3.32184500512478	-3.35261900410233
H	-5.19812099505942	3.95588199734205	-2.03375300038151
P	-5.82421097699673	-1.01325969680433	-2.02023595502090
P	1.89523630577737	4.43981302626604	-1.97975178446257
P	1.91318212216312	-1.00995888747382	-2.01667061504837
P	1.89775184229370	-6.44301302929840	-2.03802970470513
H	1.25801798696391	9.42653699189610	-1.97878100330986
H	-7.11382100001316	1.17212200803238	-0.11476399974393
H	7.01408297718646	1.19452696010285	-0.07898900851871
P	-0.03125152154172	-9.22731027888840	-0.13275298208678
P	-0.02226002088262	7.20695100231341	-0.07555247591138
P	0.00384238327311	1.75807901274448	-0.14575782836393
P	-0.04557211475899	-3.69688168305172	-0.14895591260492
H	-3.27797699348205	6.63003800053130	-0.06673200008245
P	-3.91374611687827	1.71361065195181	-0.16626851240585
P	-3.96118547842667	-3.70844303316357	-0.08546747927608
H	3.16076499684195	6.64024999474472	-0.05042600138134
P	3.76377484223782	1.75191332666743	-0.08168493208654
P	3.87161989529642	-3.69704938055540	-0.09064226650840
H	-5.20697900230587	4.14883899916979	1.85423200034905
P	-5.90402894333176	-0.85766814676030	2.10148846176599
P	1.86690453546493	4.59527549057781	2.14598376814283
P	1.88500735764196	-0.92122618298891	2.02331938364929
P	1.92886155942984	-6.27503978915970	1.98680973704644
H	1.23712802574314	9.61177001359025	1.91220400550132
O	-3.33718011340476	-3.39503853106367	3.31922916905675
O	-0.79894521994203	-3.37775103721480	3.28695174054587
H	-1.97340966149119	-0.11651980190391	2.78082320684097
H	-3.63549613581247	-3.06951906092898	4.18345973076471
H	-1.86159906843712	-3.40969725221213	3.31979775995833
H	-0.47904143290059	-4.28291008606172	3.42864643226643
H	-1.99086040662220	5.18375957449718	2.93968887024179
O	0.09504001434589	1.61232411512987	3.21900829399758
H	0.18411215253373	1.87533471415337	4.15010494450124
H	0.68984139199874	0.83677728349647	3.07702761484631
O	0.13809615746316	7.36291429549706	3.31438360849182
H	0.72567863915162	6.60279362788507	3.10425601985550
H	-0.69737210328231	6.97331331809597	3.61640871804992
O	3.81147021392560	1.79123266154367	3.28415320864200
H	3.16799889412326	1.06831985127888	3.13367139094105
H	4.67146899433101	1.33806535743653	3.37447557935350

O	3.57355090710674	-3.54428526396307	3.37780454999880
H	3.10187698911356	-4.37447781241370	3.15093894733347
H	4.36753851534211	-3.81576842810203	3.86903186360140

Explicitly solvated surface without H₂O + H⁺

Energy=-8648.0943753724

H	-1.96477200414922	5.17672299737412	-3.17568799210709
H	-1.95601009060855	-0.27005203230325	-3.21467295398781
H	-1.94724512916076	-5.71813412457536	-3.25163495338523
H	5.74729102978292	-0.25887700949852	-3.21618800811985
H	-1.15755700635482	-10.08739000784116	-0.15201197647247
Ga	-1.91030749144373	5.84715452237049	-0.02433059839494
Ga	-1.94726631307299	0.48553973610641	-0.16811376877264
Ga	-1.95293623101045	-5.04849484149517	0.00808125068043
Ga	5.71100831563397	0.39078049943503	0.05447445356641
H	4.97907595959657	-4.63355899595712	-0.11597701044134
H	-5.80765704939156	-0.27775702903483	-3.21077495852501
H	1.88687700697984	5.18301599680834	-3.17749299424612
H	1.89563901564354	-0.26375903271446	-3.21647795864074
H	1.90440310001091	-5.71184013994395	-3.25343992660523
H	-6.95352895339517	-1.87756593833880	-2.05184102095061
H	6.89939997690107	-1.85493298189561	-2.05832900363053
Ga	-0.00832014894198	3.06693119338535	-2.12214425795857
Ga	-0.00729321344592	-2.38598522886881	-2.13163900794978
Ga	-0.02645866260058	-7.88585604388487	-2.14218152874946
Ga	-0.04187908389007	8.52341641823242	-2.07116296229681
Ga	-3.90983875396313	3.06238350982892	-2.12396563655285
Ga	-3.91401848170419	-2.43125826936362	-2.11735686739346
H	-3.09193488192510	-7.31739389790380	-2.09244204086960
Ga	3.84388799707635	3.04363990294519	-2.09722123105525
Ga	3.85380325403377	-2.41131009718659	-2.12763716945688
H	3.05532885878284	-7.30735286910166	-2.09532103812893
Ga	-5.78860475599541	0.35331988668270	0.07974362175438
H	-5.02243776605393	-4.64990082593677	-0.11129003382800
H	1.13170901805974	-10.08365000919006	-0.15308499697569
Ga	1.86736923279545	5.80258273306814	0.01713824790979
Ga	1.90374258073175	0.33661259013515	0.02734304217288
Ga	1.92613572334723	-5.03639406694292	-0.04113632881361
H	-6.98058495405065	-1.64775797675212	1.65975400528781
H	6.92919401657246	-1.62503199601111	1.65323799155868
Ga	-0.02404544976725	3.38760809720563	1.55676150976296
Ga	0.00985725409927	-2.29822943494042	1.86924386730537
Ga	-0.02707733613625	-7.53487625844855	1.56566820759640
Ga	-0.04195390222694	8.73878312604647	1.68294959601367
Ga	-3.81680382841210	3.45437677598038	1.50096209558680
Ga	-4.02571921073480	-2.25584723322923	1.79453884515596
H	-3.11879505420391	-7.08761705613964	1.61952600366461
Ga	3.79000772744110	3.28844096790424	1.68785739448152
Ga	3.88695206521199	-2.18589467385827	1.76229716708234

H	3.08492697878336	-7.07748198417424	1.61661899283468
P	-1.94776277589237	4.40995346546110	-1.97876817915812
P	-1.96958109959394	-1.02370350404513	-2.02080126815301
P	-1.95783247033135	-6.45142331918566	-2.02316751801133
H	-1.36138899935145	9.40679800182720	-1.97414500052565
H	5.11235497197046	3.95690198537026	-2.01607201204686
P	5.75523231783054	-1.00256715940644	-1.99640554819453
P	-1.91705528896577	4.59668899302905	2.11880472788849
P	-1.99182809150913	-0.98869583551702	1.67283729591679
P	-1.98952526951695	-6.31195540920127	2.02491844410819
H	-1.34912298950701	9.59185400176505	1.91695499953614
H	5.11256899893404	4.14964500804237	1.87200599987922
P	5.80940169589009	-0.86005097054631	2.09165722197098
H	-0.01654298037667	-8.77734896533208	-3.37627007249079
H	-0.04280200114124	7.53512899734746	-3.29938300017892
H	-0.03404800162738	2.09598000042085	-3.32739799878883
H	-0.02528798426371	-3.34746502968504	-3.36125706784347
H	-3.88569099117814	2.08440898639196	-3.33297099721710
H	-3.87694197443734	-3.34981204014165	-3.35393897313553
H	3.81760701663052	2.09699501350710	-3.33657798615851
H	3.82635600938537	-3.33722499502675	-3.35754699760097
H	-5.18518900431154	3.94007600306384	-2.01124898721925
P	-5.81258722659551	-1.02064046314038	-1.98874119177769
P	1.89903561367038	4.42200582829287	-1.97861883371414
P	1.91885540438735	-1.00524733698485	-1.99994898507477
P	1.91131371521649	-6.45587749565428	-2.03498963064340
H	1.27098700008815	9.41109799996448	-1.97537899905256
H	-7.09505909734552	1.15609000189873	-0.08662304928703
H	7.03299294352723	1.17917296783214	-0.09323999136858
P	-0.01253859569560	-9.24147403862345	-0.12516629522021
P	-0.01719047309583	7.19381056995954	-0.07569865344218
P	0.00475779641454	1.74415229507450	-0.10535793391404
P	-0.01942471649403	-3.67947519894724	-0.11360659476724
H	-3.25920798782210	6.61424698605146	-0.04982999732694
P	-3.88640750757939	1.74934008035547	-0.09754904419656
P	-3.93196669650054	-3.73656707207032	-0.08309310078314
H	3.17960200426253	6.62476800351521	-0.05284500118766
P	3.78465959715178	1.73507137971012	-0.09379136882655
P	3.88925719860123	-3.71467510714460	-0.09850955856939
H	-5.18238099435177	4.13282399454934	1.87682699881838
P	-5.88687541149803	-0.86806355049914	2.13422500825401
P	1.87193238307028	4.56834663788749	2.13154698238580
P	1.92224554749717	-0.90965218473476	2.06476324559286
P	1.95418913811569	-6.29024519561407	1.98678781750967
H	1.26176998745359	9.59612099526197	1.91573300180191
O	-3.27000191907990	-3.40412492832097	3.34447346531883
O	-0.65169162828236	-3.33239660515104	3.36190781853514
H	-2.04858400700740	-0.14644342583201	2.80139457454801
H	-3.60265483752822	-3.19481196291987	4.23182603398565

H	-2.24245656208836	-3.41064279830712	3.38352729731749
H	-0.29485430081399	-4.23088570867609	3.43063813400190
O	-0.03305274496579	7.27977742518224	3.29842233519914
H	0.72519807361961	6.66648537036471	3.18588912156739
H	-0.81172219899997	6.68936087371957	3.22007507949973
O	3.88888899361728	1.80533065575876	3.27960787574134
H	3.17710349186938	1.13625912572730	3.19132066122694
H	4.71597678453313	1.28522288648358	3.26824089048649
O	3.60284850655185	-3.56916217907023	3.36873348273168
H	3.09898814740129	-4.38338256350190	3.15472978642642
H	4.40426787796278	-3.86483949580483	3.83194825586356

Adsorption energy study on implicitly solvated, negatively charged cluster (charge -1)

1) PyH⁺

Energy=-8514.67440297

H	5.777415	18.487199	2.804549
H	5.777415	13.040463	2.768330
H	5.777415	7.592420	2.734137
H	13.480635	13.039053	2.770423
H	6.558597	3.223509	5.836275
Ga	5.803771	19.130349	5.973957
Ga	5.772759	13.681600	5.976482
Ga	5.776576	8.162649	6.002802
Ga	13.465670	13.686070	6.032584
H	12.703926	8.667262	5.872425
H	1.925805	13.039052	2.770425
H	9.629025	18.487199	2.804549
H	9.629025	13.040463	2.768331
H	9.629025	7.592421	2.734135
H	0.776825	11.441726	3.929608
H	14.629614	11.441726	3.929608
Ga	7.703206	16.360308	3.866511
Ga	7.703236	10.921851	3.837543
Ga	7.702522	5.362759	3.898918
Ga	7.703203	21.847517	3.882261
Ga	3.826916	16.361658	3.866979
Ga	3.828210	10.882590	3.857634
H	4.629620	5.995641	3.893577
Ga	11.579575	16.361660	3.866919
Ga	11.578356	10.882476	3.857739
H	10.776820	5.995639	3.893577
Ga	1.940855	13.686333	6.032893
H	2.702513	8.667261	5.872425
H	8.847842	3.223509	5.836276
Ga	9.602840	19.130524	5.973158
Ga	9.633510	13.682007	5.976566
Ga	9.630267	8.162277	6.002244
H	0.748401	11.673463	7.640989
H	14.658040	11.673463	7.640990

Ga	7.703160	16.702711	7.505914
Ga	7.704097	11.173713	7.444625
Ga	7.703020	5.490734	8.055476
Ga	7.703261	22.193384	7.447271
Ga	3.912545	16.745848	7.483556
Ga	3.750369	11.200520	7.547601
H	4.601391	6.227347	7.605333
Ga	11.494182	16.746194	7.482450
Ga	11.654205	11.202045	7.547714
H	10.805050	6.227346	7.605333
P	5.784274	17.721412	4.003063
P	5.759598	12.298059	3.982903
P	5.781589	6.832842	3.949222
H	6.387046	22.716843	4.004203
H	12.851941	17.256424	3.968078
P	13.483449	12.291356	3.987681
P	5.815340	17.889032	8.109334
P	5.759049	12.356071	8.000104
P	5.734874	6.997703	8.018629
H	6.397786	22.903858	7.895129
H	12.850643	17.451142	7.855972
P	13.551696	12.452218	8.090277
H	7.703220	4.530028	2.611961
H	7.703220	20.842372	2.680562
H	7.703220	15.403267	2.655311
H	7.703220	9.959863	2.624217
H	3.851610	15.397984	2.647936
H	3.851610	9.963811	2.629728
H	11.554830	15.397984	2.647937
H	11.554830	9.963812	2.629729
H	2.554501	17.256422	3.968078
P	1.922943	12.291402	3.987716
P	9.622181	17.721331	4.002877
P	9.646837	12.298111	3.982996
P	9.624643	6.832436	3.948863
H	9.019394	22.716843	4.004203
H	0.639266	14.476572	5.893177
H	14.767174	14.476573	5.893176
P	7.703394	4.088419	5.937175
P	7.703222	20.482394	5.903613
P	7.702991	15.023019	5.890541
P	7.703553	9.531452	5.795638
H	4.483849	19.928409	5.929001
P	3.871907	15.031993	5.896948
P	3.822261	9.540084	5.865919
H	10.922592	19.928410	5.929001
P	11.534681	15.031876	5.896528
P	11.584074	9.540247	5.866221
H	2.555797	17.451141	7.855972

P	1.854480	12.452291	8.090602
P	9.591488	17.889852	8.106930
P	9.646594	12.359572	8.002375
P	9.671379	6.997619	8.018455
H	9.008653	22.903858	7.895129
C	6.455101	16.179935	11.215895
C	6.476116	15.032571	10.441702
C	8.853150	15.045625	10.416689
C	8.877153	16.193051	11.191067
C	7.667185	16.762621	11.599071
H	7.668668	17.660387	12.205668
H	9.826568	16.631347	11.466841
H	9.728105	14.520712	10.057027
H	5.599794	14.498304	10.099907
H	5.506775	16.607504	11.511788
N	7.663768	14.504951	10.075509
H	7.660349	13.641585	9.526571

2) CO₂

Energy=-8454.55378428583

H	5.77741496823906	18.48719903564662	2.80454899898814
H	5.77741497347468	13.04046302532028	2.76833000715261
H	5.77741498947584	7.59241994907722	2.73413703777838
H	13.48063497173559	13.03905303342252	2.77042297804433
H	6.55859696608339	3.22350892907289	5.83627499289411
Ga	5.80378753337572	19.12261436842318	5.98956209120335
Ga	5.77384629940834	13.68368596477658	5.98613222459735
Ga	5.78249580604843	8.16644739860715	6.00304160419626
Ga	13.46295390779734	13.68795889030772	6.03466232806691
H	12.70392597030192	8.66726207072218	5.87242503088647
H	1.92580501319358	13.03905202032715	2.77042499641149
H	9.62902501691674	18.48719904099518	2.80454898800970
H	9.62902502331978	13.04046299936045	2.76833100109219
H	9.62902500395401	7.59242099433118	2.73413495210017
H	0.77682500316350	11.44172599918626	3.92960800631496
H	14.62961402434169	11.44172596055713	3.92960800590804
Ga	7.70314432366221	16.35468225837975	3.87354703792900
Ga	7.70324661881675	10.92155230313693	3.84142637534601
Ga	7.70272782473862	5.36252996160614	3.89893459472866
Ga	7.70322666956591	21.84370472095835	3.88692304816717
Ga	3.82951455054860	16.36086095680825	3.87054112790620
Ga	3.83218771552881	10.88470629549111	3.85691798389131
H	4.62962004540819	5.99564104233152	3.89357699672815
Ga	11.57698907145467	16.36085019859684	3.87059051953217
Ga	11.57471317841304	10.88461744985352	3.85689218118347
H	10.77682098117700	5.99563901173136	3.89357702039306
Ga	1.94361506712587	13.68817449326393	6.03464680752071
H	2.70251299435554	8.66726101903088	5.87242500391501
H	8.84784099968169	3.22350902650469	5.83627601148395

Ga	9.60255738058447	19.12268658422833	5.98919047598224
Ga	9.63249575025817	13.68362140550067	5.98571988230654
Ga	9.62402937936692	8.16630304304503	6.00290710722390
H	0.74840102969865	11.67346300710584	7.64098900546381
H	14.65803992278545	11.67346302192839	7.64099000533397
Ga	7.70359887986607	16.65529028821774	7.55048556331710
Ga	7.70331673479651	11.19583705100952	7.46512347834436
Ga	7.70322479145336	5.49417501796887	8.05958619875173
Ga	7.70324404406464	22.19131547258221	7.44570963883001
Ga	3.91243671718651	16.73532522446035	7.49825960274750
Ga	3.75678702984213	11.19779851117017	7.53394985728969
H	4.60139098600963	6.22734701942425	7.60533300831324
Ga	11.49415945518468	16.73508620291034	7.49804673690984
Ga	11.64945748797212	11.19805495888724	7.53401059189017
H	10.80505004614647	6.22734599524678	7.60533303379235
P	5.78566888020633	17.72234176884282	4.00525097390827
P	5.76038917986233	12.30042871276509	3.98472035841822
P	5.78212643810030	6.83337004059790	3.94911027315910
H	6.38704587150557	22.71684306441602	4.00420302356721
H	12.85194105100658	17.25642407838373	3.96807803036461
P	13.48312806734469	12.29134941496761	3.98820556651207
P	5.81642331477330	17.88140178115382	8.10991838633774
P	5.74335411789351	12.36128219555543	8.00808445501295
P	5.73273440105121	6.99917399608675	8.01951961784421
H	6.39778603886161	22.90385800995610	7.89512899369143
H	12.85064305252899	17.45114200911431	7.85597204345730
P	13.54730946345245	12.44621793796898	8.08726965182566
H	7.70321999149230	4.53002800441802	2.61196093226755
H	7.70321998472365	20.84237189507585	2.68056191917205
H	7.70321999500569	15.40326595991897	2.65531095958816
H	7.70322000352466	9.95986296252226	2.62421697026964
H	3.85161003878339	15.39798393651893	2.64793597402629
H	3.85161001028687	9.96381100412570	2.62972801636721
H	11.55482996636157	15.39798390790351	2.64793692383318
H	11.55482997593912	9.96381201569597	2.62972901621182
H	2.55450094135347	17.25642204468408	3.96807802076202
P	1.92339095352288	12.29129123364900	3.98814352914390
P	9.62074565654067	17.72223507628350	4.00517525109354
P	9.64621465201714	12.30022260834207	3.98460202318454
P	9.62405773373750	6.83309198085669	3.94893226005601
H	9.01939413941478	22.71684309521703	4.00420303393889
H	0.63926595673317	14.47657200171093	5.89317698704704
H	14.76717404674493	14.47657302149679	5.89317599539195
P	7.70316170682470	4.08768260453909	5.93713578226467
P	7.70316928724143	20.47946644882816	5.90449973186575
P	7.70320989277686	15.02158084920932	5.88692490264087
P	7.70329196118449	9.54480480766489	5.80984194818656
H	4.48384918463966	19.92840884353407	5.92900103705484
P	3.87135858284509	15.03301276027440	5.89603213649571

P	3.82326445557361	9.53591435495438	5.86073909152150
H	10.92259289233326	19.92841092462649	5.92900102601783
P	11.53513401759980	15.03279368716023	5.89594835444634
P	11.58318478925655	9.53592639688643	5.86070371040200
H	2.55579694997210	17.45114101871411	7.85597201795545
P	1.85910594258936	12.44622300430793	8.08715704667191
P	9.59038736644274	17.88158123566460	8.10982305284149
P	9.66291722686821	12.36180583920884	8.00823285137660
P	9.67359155556630	6.99896274982473	8.01943829832153
H	9.00865294585745	22.90385798945063	7.89512899892244
O	7.69831524979471	14.87322020048891	9.67640129981464
O	7.70660749809824	12.88416785260477	10.90677587879215
C	7.70191870959977	13.86750541243900	10.27719486943243

3) HCOOH

Energy=-8455.75813307906

H	5.77741457771092	18.48719911607540	2.80454915290348
H	5.77741486980252	13.04046303658675	2.76833013742700
H	5.77741495280708	7.59241997631940	2.73413696117146
H	13.48063500949942	13.03905301625993	2.77042300420999
H	6.55859694532915	3.22350893273150	5.83627500652617
Ga	5.80115412252846	19.11772209949789	5.98353579748698
Ga	5.75058750294455	13.62115909366734	6.03308518685058
Ga	5.70855571043087	8.30108223963702	5.98003126666001
Ga	13.45847386647191	13.69520075853483	6.03493911382658
H	12.70392596567027	8.66726207203227	5.87242504354009
H	1.92580484274560	13.03905202149352	2.77042501577638
H	9.62902497196340	18.48719902215494	2.80454911594194
H	9.62902494308690	13.04046302450729	2.76833090467354
H	9.62902510459054	7.59242091222758	2.73413499835282
H	0.77682506606557	11.44172607214987	3.92960796406809
H	14.62961401894032	11.44172598292470	3.92960798416539
Ga	7.69749642183631	16.34133787662221	3.88510545782493
Ga	7.68939207545521	10.92656276654749	3.84383157210813
Ga	7.69367135935089	5.42588578755770	3.84782394164224
Ga	7.70314012989336	21.84215949110478	3.88879044335710
Ga	3.82582779008575	16.34508151900589	3.88594710063020
Ga	3.82424338323071	10.86550404430306	3.88453478076206
H	4.62962009843298	5.99564103885656	3.89357702038829
Ga	11.57592531987598	16.35880166223694	3.87357886755893
Ga	11.56500558407245	10.89426426657613	3.85330411993858
H	10.77682083064246	5.99563912171732	3.89357702033101
Ga	1.94209586553919	13.65541981589895	6.06383009112467
H	2.70251316676333	8.66726128358378	5.87242505923698
H	8.84784106783940	3.22350901754398	5.83627602679042
Ga	9.60255965210119	19.12091349332912	5.98278608344124
Ga	9.61681843567946	13.67340710016645	6.00107813693366
Ga	9.62354545326981	8.25618008895655	5.99158486726017
H	0.74840099091493	11.67346296200529	7.64098892627988

H	14.65803988989373	11.67346302857395	7.64098998028939
Ga	7.69739400125487	16.65816858951969	7.52305751415658
Ga	7.69405915177010	11.13386061723589	7.64477148085556
Ga	7.69697952853038	5.80294880622423	7.55016080306908
Ga	7.70317029660918	22.18966839380842	7.44449553556171
Ga	3.90786840242892	16.72073043004060	7.48633579084658
Ga	3.71587509463242	10.93978757993257	8.03587547815297
H	4.60139104247640	6.22734700594001	7.60533303594975
Ga	11.49468059022865	16.73217436817620	7.48894771308892
Ga	11.64423125728030	11.23703942867583	7.56489699191154
H	10.80504994438940	6.22734601407436	7.60533302211004
P	5.78226136888445	17.71738326978735	4.00308400465524
P	5.74887629222637	12.29448952109823	3.98475488694714
P	5.76180142254238	6.86316405778571	3.96617644437921
H	6.38704652136269	22.71684293679677	4.00420291873117
H	12.85194100673268	17.25642397151822	3.96807793268408
P	13.48263852263546	12.29162543143683	3.98899371773816
P	5.81088824067487	17.87684413833089	8.10345592356762
P	5.73045696499871	12.35471792825192	8.04405650090258
P	5.72086842736050	7.02211130230806	7.99835338759778
H	6.39778584646349	22.90385804735374	7.89512899315779
H	12.85064280826020	17.45114191510385	7.85597185640259
P	13.56194253199084	12.46009545343723	8.09355363998199
H	7.70321998910069	4.53002797137888	2.61196085268759
H	7.70321989450828	20.84237224728638	2.68056219859357
H	7.70322001983055	15.40326627690383	2.65531120449472
H	7.70322000714455	9.95986300317147	2.62421704450092
H	3.85160993366840	15.39798419468541	2.64793646762931
H	3.85160999020447	9.96381102014356	2.62972811411158
H	11.55483001026034	15.39798403914404	2.64793710901912
H	11.55483000939036	9.96381203267086	2.62972905275556
H	2.55450102462982	17.25642194733862	3.96807772030355
P	1.92487944287425	12.29100538188861	3.98888875492430
P	9.61681104184299	17.71788428620379	4.00328295721719
P	9.63845325131005	12.30117002120892	3.98579907397429
P	9.63714304098495	6.85332057763752	3.96056306806940
H	9.01939357599316	22.71684280679779	4.00420295533277
H	0.63926639234263	14.47657178359917	5.89317691180652
H	14.76717388852465	14.47657292310534	5.89317600695463
P	7.70288857439046	4.07109817194022	5.86787187603395
P	7.70163111068146	20.47759157379085	5.90391695540204
P	7.68055023714504	14.99817454165968	5.88873740742191
P	7.69118738559529	9.59848725090825	5.82493098027058
H	4.48385001903786	19.92840863704311	5.92900076328582
P	3.86874572588984	15.01327212631136	5.89795468667137
P	3.75762848634607	9.62549099974086	5.93423403552084
H	10.92259230624781	19.92841076733474	5.92900100383369
P	11.52588438548977	15.02791442033436	5.89080914489298
P	11.60165029858378	9.56263265474752	5.87987194617248

H	2.55579740572759	17.45114080419170	7.85597164217434
P	1.84074793985809	12.47062097512857	8.09361716409877
P	9.58753240083960	17.87553082609435	8.10185761071162
P	9.66270392584182	12.38641453934001	8.02302993888908
P	9.68485165873264	7.01130710185277	8.01877529796534
H	9.00865302282843	22.90385795256263	7.89512891465375
O	6.06632511845940	9.83205873521334	10.47187806053120
O	7.88734344525510	9.61622437486754	9.13889992076868
C	7.18124630758757	9.26000948294551	10.08948043389765
H	5.83707926725690	10.59548615095314	9.89245895311993
H	7.46194149105116	8.41024909010577	10.71360439211039

4) H₂O

Energy=-8342.47842731682

H	5.77741514140776	18.48719920644861	2.80454897792057
H	5.77741495919211	13.04046329815749	2.76833024218954
H	5.77741487240891	7.59241999835599	2.73413671140659
H	13.48063506708256	13.03905259624669	2.77042345260308
H	6.55859737920044	3.22350850846435	5.83627545487587
Ga	5.80342372589975	19.10324834899870	6.01480658211658
Ga	5.78813167276176	13.69980256926554	5.96070655886710
Ga	5.77967519582972	8.17046465799828	6.00742348082053
Ga	13.46084144120960	13.69167400462507	6.03075509776711
H	12.70392630544522	8.66726176694924	5.87242507054941
H	1.92580499708094	13.03905179229251	2.77042463819116
H	9.62902515958458	18.48719935214654	2.80454886358599
H	9.62902504200396	13.04046297719339	2.76833078569137
H	9.62902496536014	7.59242089551365	2.73413545866101
H	0.77682473819390	11.44172605440689	3.92960754076755
H	14.62961390172377	11.44172600832250	3.92960799296921
Ga	7.70330873672062	16.36188724885851	3.86925023747401
Ga	7.70315199565050	10.92328682715760	3.83998640441454
Ga	7.70280487366924	5.36367915042905	3.89861685647432
Ga	7.70320879036736	21.83639088083683	3.89601470208648
Ga	3.83297066603002	16.36337220806243	3.87094254801361
Ga	3.82936513630571	10.88275187327519	3.85830400608256
H	4.62962033136494	5.99564061179865	3.89357729342698
Ga	11.57356473630701	16.36333566849581	3.87100102800188
Ga	11.57743362071345	10.88289036556999	3.85821208039777
H	10.77682040794919	5.99563932683247	3.89357703287828
Ga	1.94563896988960	13.69180711124106	6.03068737900118
H	2.70251342785044	8.66726131944427	5.87242542660673
H	8.84784134000985	3.22350892202119	5.83627574150007
Ga	9.60308422242079	19.10308595650628	6.01488278588205
Ga	9.61811030010802	13.69950876689589	5.96077797230167
Ga	9.62649057109069	8.17009010678744	6.00763184112718
H	0.74840075338390	11.67346254342877	7.64098899159182
H	14.65803969906431	11.67346263403251	7.64098962292429
Ga	7.70334161413818	16.52618779021173	7.69867397744583

Ga	7.70334121727414	11.20432016322640	7.46786629706273
Ga	7.70322258063732	5.49190640935814	8.05701063863895
Ga	7.70323513487520	22.18582979928857	7.44681558118723
Ga	3.91364857819993	16.73030609796757	7.50769404815712
Ga	3.75273523231800	11.21768922500678	7.54444521196667
H	4.60139082014516	6.22734724740435	7.60533346359542
Ga	11.49289621942778	16.73003459813988	7.50769429510208
Ga	11.65355790818907	11.21750874915788	7.54441530910518
H	10.80504975234357	6.22734634768682	7.60533300402159
P	5.78608199241333	17.72533906261095	4.00726722340923
P	5.75870871837390	12.29675827865069	3.98152650498597
P	5.78137786368561	6.83558784468971	3.95056413686365
H	6.38704552608372	22.71684350402609	4.00420323623246
H	12.85194061994267	17.25642352942847	3.96807751997282
P	13.48369819618109	12.29138605153403	3.98807985267757
P	5.82245332516083	17.85645601354926	8.11828374573047
P	5.75346235658169	12.38439434413624	8.00315925545877
P	5.73275205837092	6.99950356421441	8.02075956479807
H	6.39778582214772	22.90385777614718	7.89512880351575
H	12.85064290369984	17.45114194391416	7.85597213401691
P	13.55563662237020	12.45631815797833	8.09017049367830
H	7.70321979522895	4.53002829101417	2.61196071634709
H	7.70321993734476	20.84237156364982	2.68056172470423
H	7.70322001655193	15.40326642784269	2.65531102257443
H	7.70321995007730	9.95986314510250	2.62421698801717
H	3.85160999739039	15.39798405913156	2.64793624545076
H	3.85160997632304	9.96381132396191	2.62972782667147
H	11.55483006087302	15.39798442384834	2.64793746906571
H	11.55482988226212	9.96381196394975	2.62972867749255
H	2.55450159654241	17.25642169750677	3.96807761655649
P	1.92281937001971	12.29127456737657	3.98801113957472
P	9.62047112940311	17.72533139793170	4.00724483756039
P	9.64769600129665	12.29658509481233	3.98152261504868
P	9.62475460710070	6.83536943394773	3.95042202272429
H	9.01939458040779	22.71684281576022	4.00420266973227
H	0.63926622681936	14.47657192351280	5.89317720672295
H	14.76717415780784	14.47657322107154	5.89317634063045
P	7.70323773354230	4.08786110411496	5.93575404648258
P	7.70328228462540	20.46757797395825	5.91325016484658
P	7.70321087785036	15.04829055851755	5.86838761466450
P	7.70318279170837	9.55000254403510	5.81412117876413
H	4.48384884588882	19.92840938874133	5.92900070278020
P	3.87229201583629	15.03255544764660	5.89548311868429
P	3.82143544118839	9.54420254434323	5.86963228974931
H	10.92259274221625	19.92841069010643	5.92900141278147
P	11.53406334552194	15.03229025327434	5.89549112083830
P	11.58486296683795	9.54379439540277	5.86945773295422
H	2.55579683578111	17.45114100975556	7.85597162676570
P	1.85069344418759	12.45648948912311	8.09019316862320

P	9.58413836998756	17.85637522261764	8.11824356770416
P	9.65309589815054	12.38417986759179	8.00368463171137
P	9.67341659538884	6.99900902570916	8.02084130301440
H	9.00865307779779	22.90385829065447	7.89512908854453
O	7.70285639269713	14.98599262856432	9.25886609518719
H	8.47304356419908	14.38389673312407	9.18758868480335
H	6.92769619682902	14.38956376468676	9.19155755244020

5) o-DHP

Energy=-8515.40665383567

H	5.77741510923516	18.48719911557479	2.80454893116755
H	5.77741497999929	13.04046328264239	2.76833018487609
H	5.77741484885467	7.59241999429285	2.73413669812520
H	13.48063529548486	13.03905249031483	2.77042346154098
H	6.55859728950649	3.22350856467136	5.83627544714465
Ga	5.80278949963176	19.12124472428289	5.98356399466122
Ga	5.78359977497862	13.66210283498222	5.98471684833759
Ga	5.80411620970063	8.18694852518884	5.98952895685333
Ga	13.45686023639049	13.69660676106111	6.03340120637590
H	12.70392641853924	8.66726174770523	5.87242513884822
H	1.92580486306922	13.03905173030197	2.77042465074359
H	9.62902516224565	18.48719926860888	2.80454881464484
H	9.62902504301795	13.04046297847021	2.76833073067371
H	9.62902496788795	7.59242090025928	2.73413542132479
H	0.77682484609897	11.44172612111169	3.92960749659330
H	14.62961372735950	11.44172616101897	3.92960797552863
Ga	7.70439627079064	16.35137443242993	3.87603460495463
Ga	7.70338687029736	10.90885690295602	3.86073026046512
Ga	7.70450441588040	5.37301528555402	3.89179189892233
Ga	7.70321853590808	21.84334980993715	3.88732839958949
Ga	3.82706300504506	16.35598761144686	3.87476466147679
Ga	3.83857363958695	10.87989999404832	3.86497601633033
H	4.62962034811642	5.99564063342967	3.89357729320138
Ga	11.57750790381691	16.35833653373961	3.87301403325322
Ga	11.57056747885053	10.88401193544542	3.86090770001449
H	10.77682039520683	5.99563932544105	3.89357702836328
Ga	1.94420786454504	13.68620251227373	6.03415937828519
H	2.70251338824022	8.66726127311390	5.87242543040247
H	8.84784145586665	3.22350884884067	5.83627573351997
Ga	9.60289001449742	19.12287644380858	5.98451013860857
Ga	9.62326134322101	13.65954491210337	5.98849543260445
Ga	9.59911712525798	8.18991104068492	5.99908646124941
H	0.74235901979157	11.64697399993406	7.64093316110443
H	14.65193834003138	11.67486483692078	7.61113869440757
Ga	7.70324390459358	16.66480372719281	7.52815941018661
Ga	7.68890396719735	11.09937568283129	7.70990694288080
Ga	7.70981542526701	5.46376320078432	8.03048306801842
Ga	7.70321451159947	22.19081628132732	7.44485494477115
Ga	3.90916124204545	16.72715705374661	7.48681566097315

Ga	3.77902972128191	11.22932388035422	7.54776703763506
H	4.60139078986328	6.22734721814476	7.60533345894053
Ga	11.49541395450408	16.73128036385038	7.48878747220623
Ga	11.63536605624057	11.22402630049331	7.52985893301108
H	10.80504969877477	6.22734639945501	7.60533303846458
P	5.78510554532900	17.71953975908752	4.00331414346522
P	5.76412946850247	12.29603719741368	3.98063699152497
P	5.78164798059927	6.83702916365884	3.94913944106283
H	6.38704562623695	22.71684346750767	4.00420320929025
H	12.85194054913589	17.25642345709856	3.96807746469748
P	13.48231746784264	12.29105858029692	3.98889901507527
P	5.81263633320147	17.87740660982412	8.10375449499456
P	5.74454866123773	12.41336972703593	8.01056823464026
P	5.75697291821802	6.97313029513289	7.98229428718860
H	6.39778599758196	22.90385779888146	7.89512875062277
H	12.85064297186181	17.45114198512582	7.85597215135669
P	13.55082937160658	12.44539017561604	8.07953709309015
H	7.70321981173324	4.53002833076348	2.61196077765142
H	7.70321998459751	20.84237172358371	2.68056187528464
H	7.70322005803547	15.40326656806160	2.65531096188431
H	7.70321995360021	9.95986324894795	2.62421712667029
H	3.85161004095336	15.39798402372804	2.64793618033533
H	3.85160995166338	9.96381140294907	2.62972785832562
H	11.55483010044763	15.39798453797266	2.64793753232838
H	11.55482982356031	9.96381203823307	2.62972865626082
H	2.55450152959700	17.25642176644559	3.96807764669308
P	1.92553658118868	12.28852471747858	3.98756234105595
P	9.62115925572725	17.72134509399574	4.00357631727962
P	9.64331333737297	12.29557440929787	3.98086453140664
P	9.62508907176471	6.83868136848768	3.95173021711082
H	9.01939441120829	22.71684272647231	4.00420262731019
H	0.63926655177994	14.47657183002693	5.89317724269373
H	14.76717388422961	14.47657309368326	5.89317634616657
P	7.70402230345049	4.08538564142667	5.92342027872538
P	7.70255522057213	20.47911742602475	5.90374843593968
P	7.70429134293362	15.01600890822461	5.88198686812681
P	7.69942377908865	9.60007823623791	5.85327254091097
H	4.48384893588749	19.92840931109434	5.92900073657988
P	3.87660051031249	15.02394013699630	5.88875818559010
P	3.82591001122710	9.53970817555733	5.87921743569473
H	10.92259266873377	19.92841062546673	5.92900143008965
P	11.52446461650623	15.02834215564200	5.88920311360876
P	11.58004670382491	9.53734033318420	5.87054139774841
H	2.55579672568877	17.45114109354666	7.85597166422585
P	1.84502270676587	12.43434687297566	8.08514665030597
P	9.59172831997136	17.88005200285075	8.10549504678862
P	9.66083408058212	12.38484491024766	8.00859015612511
P	9.66048082646058	6.98914520120256	8.00194918269944
H	9.00865292360908	22.90385824877703	7.89512906780887

C	6.21328945636029	10.75117887485971	11.06859386428999
C	6.35516133215032	9.82218137864568	10.11152674989196
C	8.78689558198465	9.91055413501155	10.33739025370220
C	8.59650761385797	11.20393925315127	11.08965742015454
C	7.35645447559790	11.57844062175240	11.45165562090769
H	7.18369623846211	12.47925245538500	12.03218271535360
H	9.47720545869766	11.77075044227381	11.36904913095153
H	8.85739205072473	9.06142067084736	11.03310686810210
H	5.56600664120572	9.19025715354154	9.72528922894225
H	5.24606780350090	10.90542886104459	11.53298847846067
N	7.62298616695021	9.69670747685587	9.42545971076478
H	7.69501173215650	8.75963454367927	9.02599203236811
H	9.69138189456076	9.91895057346879	9.72741421915567

6) Py

Energy=-8514.2347405538

H	5.77741511685321	18.48719923801997	2.80454892599094
H	5.77741498691068	13.04046329022455	2.76833017855782
H	5.77741485029567	7.59242001583165	2.73413669065039
H	13.48063514787597	13.03905253453568	2.77042348218689
H	6.55859747419800	3.22350849612151	5.83627544080013
Ga	5.80449892141199	19.10946478248982	5.99799321737266
Ga	5.79858046102214	13.69596415361688	5.99788186442951
Ga	5.78297169409301	8.17007812233324	6.00118142211899
Ga	13.45775803508257	13.69406876895272	6.03867907958108
H	12.70392629349574	8.66726174871408	5.87242508017087
H	1.92580486704398	13.03905168403734	2.77042473167636
H	9.62902517856035	18.48719935410732	2.80454880681083
H	9.62902502623658	13.04046298931000	2.76833074836387
H	9.62902497650736	7.59242093141041	2.73413542078452
H	0.77682484919767	11.44172616741632	3.92960746356498
H	14.62961381646359	11.44172608216620	3.92960797753539
Ga	7.70312572812886	16.34135851465145	3.89511823668483
Ga	7.70294995222283	10.92624547678476	3.83971434188157
Ga	7.70277865350975	5.36360499961854	3.89829533081449
Ga	7.70316018662041	21.83865449097092	3.89352665940418
Ga	3.83478810409949	16.36151995121200	3.87460553063121
Ga	3.83661900280274	10.89037042054213	3.85491809586100
H	4.62962036944790	5.99564063383026	3.89357730199589
Ga	11.57181698364758	16.36120480073820	3.87495204207597
Ga	11.56919647593599	10.88991657543021	3.85510562017197
H	10.77682040574947	5.99563931712855	3.89357706033149
Ga	1.94921135536214	13.69504537347216	6.03967683247781
H	2.70251342539876	8.66726130680026	5.87242541464600
H	8.84784125265345	3.22350895986004	5.83627574120461
Ga	9.60195258391531	19.10949423525052	5.99709784789804
Ga	9.60796906126355	13.69607760862224	5.99766618538800
Ga	9.62319559935581	8.17006199091162	6.00039062426644
H	0.74840066161871	11.67346250565256	7.64098897140171

H	14.65803972598111	11.67346263107529	7.64098961390236
Ga	7.70331372226889	16.55974485955445	7.77081387043208
Ga	7.70299332540885	11.19977779740825	7.46382199820251
Ga	7.70342819388895	5.49555977460395	8.05465436741612
Ga	7.70324862100351	22.18685553273766	7.44300553714359
Ga	3.91990478762982	16.75205463469619	7.49347417961082
Ga	3.76851435642262	11.20306816103054	7.52010587836689
H	4.60139087755823	6.22734725200571	7.60533347697562
Ga	11.48648182991412	16.75208504733990	7.49331791003878
Ga	11.63786281556701	11.20302189604071	7.51974693458975
H	10.80504969414225	6.22734636198197	7.60533301352342
P	5.78927190620135	17.72167154443266	4.00523866758328
P	5.76268179501443	12.30819311327185	3.98966999163700
P	5.78208900620985	6.83337433738021	3.94912066296016
H	6.38704562678579	22.71684346697884	4.00420320344257
H	12.85194067763245	17.25642362534368	3.96807758812946
P	13.48258157074828	12.29250174562016	3.98931198145819
P	5.81162645717895	17.90237033928557	8.10137673853239
P	5.74515262142965	12.35903818889948	8.01577611819379
P	5.73295639766940	7.00007127083909	8.01685940249593
H	6.39778599286980	22.90385780538046	7.89512874413389
H	12.85064297052669	17.45114206340051	7.85597212236042
P	13.54193472229655	12.44154312461061	8.08368736187544
H	7.70321976632129	4.53002823907725	2.61196071790021
H	7.70321998286507	20.84237175133257	2.68056189984078
H	7.70322003691953	15.40326647800484	2.65531101469463
H	7.70321993896685	9.95986320835337	2.62421713812907
H	3.85161006559273	15.39798398169662	2.64793622270806
H	3.85160993710283	9.96381141532592	2.62972789013221
H	11.55483002359003	15.39798433485013	2.64793737164064
H	11.55482989918694	9.96381198621834	2.62972866469016
H	2.55450145713888	17.25642180527297	3.96807762620450
P	1.92349993617389	12.29304006858433	3.98959019930670
P	9.61719141489958	17.72146202394274	4.00507524302226
P	9.64349046665293	12.30809951034335	3.98966481835326
P	9.62396031373546	6.83304367027958	3.94889414357349
H	9.01939440290212	22.71684271926373	4.00420262617344
H	0.63926651359742	14.47657180582666	5.89317718865592
H	14.76717404425680	14.47657315460948	5.89317634337366
P	7.70315282977010	4.08805432545146	5.93523769729218
P	7.70320019346327	20.47427101626221	5.90504703126398
P	7.70319046028317	15.06616161622337	5.92819327013970
P	7.70299863775852	9.54546445934034	5.80703484550586
H	4.48384915728459	19.92840922631736	5.92900070959193
P	3.87956838202025	15.03303087481406	5.90385220659583
P	3.82357201849007	9.53416253779042	5.85628953501613
H	10.92259249410748	19.92841049824175	5.92900145810582
P	11.52727017780152	15.03265102033611	5.90411168357393
P	11.58279655572848	9.53391252402328	5.85602798499449

H	2.55579671896852	17.45114108096911	7.85597165966857
P	1.86431232107568	12.44130518559413	8.08403603267127
P	9.59479019125450	17.90308572725055	8.10028622256931
P	9.66108873857197	12.35834759721963	8.01504441059442
P	9.67358081761308	7.00078473651852	8.01536959520728
H	9.00865291446975	22.90385824957943	7.89512906388189
C	8.90716597453753	14.16821304028161	11.24698528863991
C	8.86486217620103	14.93674595854753	10.09062004697040
C	6.54364191404244	14.93514226927950	10.08971472541263
C	6.50157291013888	14.16650269583804	11.24602449921049
C	7.70440783150688	13.77828860361656	11.83764850736707
H	7.70444967163314	13.17943001288171	12.74193656996039
H	5.54599319483078	13.87137777699660	11.66250359418693
H	5.63963579237471	15.26628965542556	9.59372786380257
H	9.76889676542143	15.26973171547234	9.59587619069452
H	9.86295899940987	13.87566879648259	11.66477796824180
N	7.70420524235848	15.32548624565982	9.52756407199672

7) HCOO⁻

Energy=-8455.3203440984

H	5.77741497259960	18.48719902420824	2.80454898444319
H	5.77741496425119	13.04046300855016	2.76833000792766
H	5.77741496667513	7.59241993824586	2.73413701282267
H	13.48063512441255	13.03905291079878	2.77042304149663
H	6.55859687430195	3.22350905748081	5.83627502772998
Ga	5.80241266666257	19.11911841210993	5.97984732358964
Ga	5.76301527083774	13.73072198948142	5.91219468742623
Ga	5.77551001204318	8.19383490438739	6.01886403044451
Ga	13.45683306600274	13.68780462735359	6.03791836554223
H	12.70392599990421	8.66726201935467	5.87242500287609
H	1.92580491662300	13.03905191832630	2.77042505454428
H	9.62902500212961	18.48719900343019	2.80454902719200
H	9.62902503603479	13.04046301376746	2.76833099161935
H	9.62902499100849	7.59242093708609	2.73413503834882
H	0.77682508969078	11.44172608790708	3.92960794183212
H	14.62961387223410	11.44172611995061	3.92960796221914
Ga	7.72022958040691	16.36153258361606	3.86704754429840
Ga	7.69424636903708	10.90471038889665	3.86834476348212
Ga	7.70023282349049	5.38093047613211	3.89201210951342
Ga	7.70332469346168	21.84209728033810	3.88882900219159
Ga	3.82382787109427	16.36513794204476	3.86448699902496
Ga	3.83280378994083	10.86489204127812	3.88713315999002
H	4.62962000294768	5.99564103117270	3.89357698634087
Ga	11.57775616377167	16.34490346850070	3.88682791370929
Ga	11.55979287329624	10.88140129162237	3.86636434395304
H	10.77682098149766	5.99563902462414	3.89357696970737
Ga	1.94662064514426	13.66093778694323	6.07418902134564
H	2.70251304650297	8.66726102037349	5.87242498020855
H	8.84784113829426	3.22350893955010	5.83627600145759

Ga	9.60384567729181	19.12107120417206	5.98784650783107
Ga	9.59205888556665	13.62809132464915	6.03810480425019
Ga	9.58233956186026	8.20704671663777	6.03182877817417
H	0.74840097823484	11.67346298247782	7.64098900358532
H	14.65804007005503	11.67346297687571	7.64098998828506
Ga	7.69856828667614	16.66494235244874	7.51726108295984
Ga	7.52268035853685	11.12713284924124	7.69935852357248
Ga	7.70914087241968	5.46718294975467	8.03346586007151
Ga	7.70311246423635	22.18961833458750	7.44438647888135
Ga	3.90793300021086	16.72893322748031	7.47207867691523
Ga	3.90646172932218	11.13867715274703	7.74292886071175
H	4.60139088846662	6.22734696509768	7.60533298274367
Ga	11.49491157840982	16.72334634046994	7.49054968008657
Ga	11.61103089003802	11.20328789927813	7.56646711544101
H	10.80505008570295	6.22734598442153	7.60533299056986
P	5.78892278858542	17.71772645605655	4.00012308052527
P	5.75659409292847	12.29611226498952	3.97488243590927
P	5.77768417090866	6.84336384679149	3.95751089682918
H	6.38704602976228	22.71684298001062	4.00420298695589
H	12.85194101707880	17.25642400542710	3.96807796352173
P	13.47857712598415	12.28761967539222	3.98811505273976
P	5.81019797447086	17.87847915548516	8.10167227985756
P	5.73120351857424	12.61294739936458	7.93542213193848
P	5.75964812363079	6.95326692893575	8.00213929090380
H	6.39778618906678	22.90385801585605	7.89512894595727
H	12.85064291324814	17.45114198156376	7.85597197047614
P	13.54114577455202	12.44164409737604	8.08650607673295
H	7.70322004502947	4.53002807997444	2.61196100925213
H	7.70322005864535	20.84237210025923	2.68056210377397
H	7.70322000035766	15.40326602830109	2.65531102066338
H	7.70322000219770	9.95986296123929	2.62421695605980
H	3.85160999137498	15.39798401854282	2.64793604548274
H	3.85161000715549	9.96381103933826	2.62972806968729
H	11.55482999791538	15.39798401819176	2.64793703110904
H	11.55482998766933	9.96381204125415	2.62972904161056
H	2.55450099938956	17.25642199484894	3.96807797360765
P	1.92633066947294	12.28991756833456	3.99231242818683
P	9.62963319382456	17.72551152355779	4.00318700399268
P	9.63540195735921	12.29586844330350	3.98813428249360
P	9.62576962995930	6.84581874748503	3.96021314786611
H	9.01939388089619	22.71684293236863	4.00420297100474
H	0.63926600299687	14.47657202018602	5.89317697047419
H	14.76717389485705	14.47657294726661	5.89317599976277
P	7.70506638619993	4.08810433082724	5.92400434133340
P	7.70287575624578	20.47816604057001	5.90362781304233
P	7.71236774729165	15.03633411405653	5.85750344198166
P	7.67065372287333	9.60503496010585	5.86237300486974
H	4.48384906547436	19.92840897144901	5.92900099594113
P	3.84510862461502	15.05215445500808	5.85896154628909

P	3.82015587904242	9.56296995637023	5.90483172424182
H	10.92259297719753	19.92841099719864	5.92900099613026
P	11.50847078679005	15.00251774869149	5.90732327363159
P	11.57766794333266	9.53705846125544	5.87591961905852
H	2.55579807731571	17.45114096603283	7.85597197040314
P	1.89473360785900	12.39988718371248	8.09565770003318
P	9.59064719682263	17.87640026945797	8.10535168702132
P	9.59584546763278	12.30905883733056	8.06201253040614
P	9.66391051716972	6.98621486048204	8.02171645332297
H	9.00865282218834	22.90385794167288	7.89512896721167
O	4.58899116184293	9.93222054454192	9.30105633414961
O	6.89447687498155	9.88914350450740	9.24798629654804
C	5.74614978543116	9.60640489976215	9.71901935119336
H	5.75690519203933	9.01113754208273	10.64138334455494

8) OH⁻

Energy=-8342.00486678468

H	5.77741516775948	18.48719923076242	2.80454893684391
H	5.77741502041977	13.04046332203148	2.76833020772746
H	5.77741496755444	7.59242011262416	2.73413663721153
H	13.48063502723170	13.03905262549281	2.77042344976872
H	6.55859710218899	3.22350856364298	5.83627545001316
Ga	5.80883355518248	19.10342839285279	6.01102034005676
Ga	5.81374290329254	13.72819919452225	5.98939769995571
Ga	5.78083790580435	8.17672556355043	6.00547706691191
Ga	13.45175530053862	13.70199072088951	6.03654737446805
H	12.70392629979282	8.66726174340142	5.87242502390017
H	1.92580499790550	13.03905177302849	2.77042465477037
H	9.62902513953733	18.48719936858085	2.80454884679057
H	9.62902502260484	13.04046304105215	2.76833078005437
H	9.62902486805057	7.59242098387448	2.73413540053322
H	0.77682474429688	11.44172606521009	3.92960754527847
H	14.62961391645204	11.44172598617788	3.92960800366951
Ga	7.70320106134250	16.34257195161356	3.90087773076213
Ga	7.70293024091552	10.93197499202287	3.83705778331383
Ga	7.70270870582608	5.36707816941261	3.89764462512740
Ga	7.70320430351745	21.83663498074005	3.89621897365382
Ga	3.83803940976629	16.36104011233958	3.88092553389887
Ga	3.84026737463089	10.89242687300446	3.85534353821415
H	4.62962018869860	5.99564050014638	3.89357732749060
Ga	11.56854209413220	16.36081043506030	3.88114984058095
Ga	11.56644907732534	10.89222403146005	3.85548400767497
H	10.77682051951806	5.99563922750508	3.89357705168716
Ga	1.95472396963573	13.70212095444108	6.03682179950931
H	2.70251338485644	8.66726126026892	5.87242541530664
H	8.84784162214769	3.22350883173013	5.83627574526080
Ga	9.59764479543216	19.10327109830477	6.01081163364102
Ga	9.59279677984322	13.72804027858787	5.98858820865077
Ga	9.62553036595364	8.17660527891372	6.00516059270876

H	0.74840074774865	11.67346254366729	7.64098899405905
H	14.65803966237866	11.67346265391280	7.64098963376709
Ga	7.70358939914148	16.47015412602142	7.92969400275087
Ga	7.70322812115050	11.20301325968755	7.46431367767357
Ga	7.70304175376126	5.49407987373947	8.05367091518410
Ga	7.70323811276561	22.18484248665883	7.43942529454020
Ga	3.93774729249615	16.76111431934809	7.52200946592429
Ga	3.77058957546737	11.21787803479993	7.53170929149616
H	4.60139081287104	6.22734725338645	7.60533346596037
Ga	11.46865014515798	16.76108773618505	7.52226588162774
Ga	11.63586104502934	11.21821305097629	7.53176384010700
H	10.80504977727668	6.22734636130083	7.60533300755573
P	5.79022166935909	17.72487174926725	4.00670211051600
P	5.76327158970786	12.31351991697517	3.99346353519078
P	5.78118097033081	6.83570339182466	3.95170027354066
H	6.38704562733454	22.71684344584078	4.00420320397727
H	12.85194071643992	17.25642366661720	3.96807764089508
P	13.48231191567730	12.29313405074750	3.98984635450408
P	5.83075477704694	17.91367736729085	8.10327460504584
P	5.75692000465749	12.37912406467056	8.01444809844268
P	5.73491858015663	6.99870395097063	8.01690121590702
H	6.39778594020505	22.90385778826451	7.89512876079982
H	12.85064295574068	17.45114196036233	7.85597216070888
P	13.54732588910831	12.44885492657742	8.08563991535517
H	7.70321983164089	4.53002833079796	2.61196079161126
H	7.70321997392382	20.84237172954008	2.68056189180757
H	7.70322001616134	15.40326643015182	2.65531105184901
H	7.70321992011310	9.95986314641804	2.62421709501837
H	3.85161004421660	15.39798398293190	2.64793619048882
H	3.85160993896970	9.96381134739054	2.62972781859150
H	11.55482999700504	15.39798425139112	2.64793729575364
H	11.55482991383538	9.96381189945939	2.62972867281701
H	2.55450150927391	17.25642177103455	3.96807765078354
P	1.92410306836921	12.29312652931973	3.98983624875600
P	9.61628954350852	17.72475299145172	4.00664183324338
P	9.64311118867840	12.31315652172123	3.99324830701883
P	9.62512302199700	6.83544387304546	3.95142787820244
H	9.01939442096983	22.71684272085041	4.00420262715360
H	0.63926625908902	14.47657190185807	5.89317720793169
H	14.76717420797737	14.47657324350959	5.89317634873688
P	7.70340460526998	4.08926025768529	5.93550424463414
P	7.70326468111513	20.47678758031736	5.90013256730281
P	7.70329118166223	15.10787372698639	5.94759410581323
P	7.70314678269206	9.55079512585080	5.80686789291815
H	4.48384888554220	19.92840936819249	5.92900069954095
P	3.88025490986431	15.04384046436575	5.91407790982308
P	3.82155609506881	9.54223593429777	5.86195944915318
H	10.92259271317637	19.92841067492860	5.92900140873126
P	11.52622498622815	15.04377737056245	5.91422627598071

P	11.58475129306712	9.54218789897276	5.86201370601227
H	2.55579677537879	17.45114104565884	7.85597165839269
P	1.85917562255280	12.44872007906674	8.08562473036527
P	9.57581811822067	17.91413453379193	8.10339916849706
P	9.64937398142650	12.37933441226732	8.01428363897525
P	9.67133232273576	6.99866870700264	8.01669332097786
H	9.00865297040692	22.90385825386091	7.89512907304480
O	7.70376675301550	15.29753646803764	9.43504551181303
H	7.70490791487234	14.37514920450004	9.13779207924390

9) $\text{H}_2\text{O} + \text{H}^+$

Energy=-8342.93423441058

H	5.77741506193233	18.48719917784761	2.80454898978590
H	5.77741494685367	13.04046326826334	2.76833029592981
H	5.77741499274200	7.59242014670510	2.73413663247823
H	13.48063515744227	13.03905253489461	2.77042348196604
H	6.55859721291233	3.22350850968499	5.83627544538067
Ga	5.80641692322579	19.13224924618693	5.98135354157954
Ga	5.79124594755276	13.71305478377476	5.88208380893155
Ga	5.80576135253412	8.16231696196597	5.97801969261838
Ga	13.46398212158926	13.68997311909319	6.03858575668205
H	12.70392633816845	8.66726175938757	5.87242508631588
H	1.92580491977142	13.03905178471334	2.77042456545786
H	9.62902520822223	18.48719934187417	2.80454881493572
H	9.62902511418191	13.04046301019264	2.76833071216700
H	9.62902480679173	7.59242108395047	2.73413535207534
H	0.77682475666393	11.44172603697503	3.92960753016406
H	14.62961383391920	11.44172607423674	3.92960795891858
Ga	7.71358278433912	16.36111732369355	3.86754846296389
Ga	7.73027737718917	10.92669156520445	3.82956486318225
Ga	7.70329955898610	5.36027563126269	3.89677131673719
Ga	7.70326044601818	21.84723803692394	3.88269759925049
Ga	3.82937226166118	16.36623960809484	3.86479370251711
Ga	3.81602094737602	10.88615758598561	3.84820059589137
H	4.62962017355075	5.99564048298846	3.89357732657825
Ga	11.58046487280580	16.35498108280665	3.87386973026523
Ga	11.58787221117129	10.88239226903297	3.85737410945756
H	10.77682060584437	5.99563914545975	3.89357706750507
Ga	1.94036099101660	13.68668154616212	6.02057671102470
H	2.70251347673260	8.66726135746149	5.87242544004360
H	8.84784149952024	3.22350888110269	5.83627573713202
Ga	9.60294833425130	19.12921143900251	5.98582584502012
Ga	9.63323962258366	13.64560489937949	6.01047591010327
Ga	9.62961507854349	8.16542828123969	5.96472341740306
H	0.74840063954468	11.67346250569321	7.64098896802546
H	14.65803975980495	11.67346261630230	7.64098959643871
Ga	7.70829935500988	16.68319433095607	7.54278772879501
Ga	7.87619850828717	10.95642384661685	7.65677798746071
Ga	7.71035412170281	5.46215555191110	8.04353528124959

Ga	7.70320842533432	22.19408679569031	7.44633147270344
Ga	3.91646549253031	16.74816549616639	7.50090419257275
Ga	3.61643900396960	11.12696361940771	7.56082649309976
H	4.60139079242798	6.22734721450573	7.60533346860023
Ga	11.49664283151145	16.73212439508551	7.49704131159503
Ga	11.67790833182380	11.19761495899206	7.56458443463217
H	10.80504975141134	6.22734636043086	7.60533300854337
P	5.78908636305584	17.72115934384319	4.00596735510095
P	5.76541030036658	12.27667456805597	3.96340888428605
P	5.78325336433352	6.82973855833365	3.94323680887526
H	6.38704559044279	22.71684348809121	4.00420320390413
H	12.85194064272638	17.25642361909325	3.96807756711568
P	13.48676153936868	12.29442231713994	3.99002379860086
P	5.81784885428376	17.88980167916353	8.11027581481350
P	5.77162484856021	12.13595764340212	7.75518127970233
P	5.75671067906527	6.98400376073853	7.98621691083689
H	6.39778589267536	22.90385776717564	7.89512877662017
H	12.85064302421623	17.45114201228303	7.85597214925236
P	13.56364994925977	12.45656714999657	8.09816028463823
H	7.70321980611766	4.53002831568784	2.61196086018003
H	7.70321993156569	20.84237166623326	2.68056180734593
H	7.70322006351258	15.40326646729751	2.65531095649111
H	7.70321994283083	9.95986307498381	2.62421695206253
H	3.85161014492167	15.39798381873503	2.64793601097638
H	3.85160997773942	9.96381139025294	2.62972783590055
H	11.55483002865613	15.39798435168239	2.64793740044037
H	11.55482985396975	9.96381206428554	2.62972878041339
H	2.55450137702517	17.25642190864977	3.96807773036376
P	1.91957575233275	12.29227096215118	3.98655702537410
P	9.62712077721136	17.72446234678198	4.00644477471377
P	9.65748706137479	12.29982982230733	3.98525435258605
P	9.62333493780473	6.82718730630610	3.94105338380771
H	9.01939450023117	22.71684277374660	4.00420264297433
H	0.63926657980085	14.47657186541104	5.89317728996127
H	14.76717399010611	14.47657314139892	5.89317633759615
P	7.70339526343548	4.08517836827369	5.93214311416513
P	7.70482113111171	20.48377487204683	5.90255968102249
P	7.72249817419167	15.01761439328853	5.89995211828334
P	7.71436447227114	9.56268134322251	5.77946743930521
H	4.48384906546315	19.92840924123315	5.92900074190700
P	3.87274497423840	15.02659313484507	5.90758198175928
P	3.82453910068440	9.52949059760855	5.85642963347309
H	10.92259275959820	19.92841066878075	5.92900143015857
P	11.52557597362120	15.02029267239458	5.90263011230398
P	11.58718697474785	9.54296928819570	5.87105025754285
H	2.55579641632004	17.45114121469864	7.85597177465771
P	1.82523708659407	12.47603979541380	8.10873581745810
P	9.59710006726030	17.88844531917581	8.10723781007587
P	9.68988782210824	12.36230535506668	8.06325660565380

P	9.65277138250193	6.99064592552871	7.98032764242911
H	9.00865301266731	22.90385829621643	7.89512909422754
O	7.69372371835421	9.52384219247492	9.19642192770864
H	8.45068557425004	8.90181833981517	9.25695972058382
H	6.88940899464204	8.96095900040941	9.17549703206051
H	5.72807661872181	12.98356096094689	8.87686403241374

Adsorption energy study on implicitly solvated, negatively charged cluster (charge -2)

1) PyH⁺

Energy=-8514.78891162237

H	5.77741511277242	18.48719923640938	2.80454887346472
H	5.77741500055125	13.04046335700979	2.76833020712983
H	5.77741484188880	7.59242002872335	2.73413668947929
H	13.48063504914558	13.03905261146659	2.77042344746816
H	6.55859722732764	3.22350847077238	5.83627544065457
Ga	5.80323675926493	19.12840657486811	5.97408376301714
Ga	5.77278754193151	13.67309264499169	5.97561050721975
Ga	5.79823910494267	8.11316062618517	6.04051740563952
Ga	13.46556565861466	13.68157433996111	6.03044567845046
H	12.70392627964326	8.66726175435889	5.87242507639074
H	1.92580495561991	13.03905177370156	2.77042467080929
H	9.62902517076078	18.48719934996484	2.80454877676874
H	9.62902501557054	13.04046305562924	2.76833075010447
H	9.62902495960527	7.59242096445069	2.73413537876659
H	0.77682475580788	11.44172608252551	3.92960752352222
H	14.62961391165432	11.44172599854211	3.92960800776703
Ga	7.70309528036840	16.35716073666534	3.86908498952992
Ga	7.70325170441433	10.90690999991748	3.85088635475260
Ga	7.70291506313882	5.31492803801924	3.94655207291811
Ga	7.70327272402739	21.84661527271956	3.88322908177860
Ga	3.82675205050343	16.35955088132598	3.86916696090551
Ga	3.83223762158611	10.87123190204755	3.86789441761436
H	4.62962037910757	5.99564064275207	3.89357730673977
Ga	11.57973898039110	16.35953238860012	3.86912615293990
Ga	11.57421857606218	10.87120056224353	3.86797962699086
H	10.77682041728615	5.99563930060167	3.89357707392468
Ga	1.94113655922926	13.68200920721428	6.03082425578866
H	2.70251346773110	8.66726135408802	5.87242543588654
H	8.84784147374896	3.22350891545604	5.83627575176284
Ga	9.60346988836475	19.12838024724835	5.97318756626145
Ga	9.63369869348409	13.67339744995437	5.97559843798708
Ga	9.60895721657097	8.11292415917938	6.03980246127437
H	0.74840071518412	11.67346252308270	7.64098898424260
H	14.65803966824982	11.67346265091291	7.64098962466933
Ga	7.70327150789166	16.69841710468160	7.50215320669575
Ga	7.70426499572149	11.15958393964822	7.43798163854233
Ga	7.70410957210130	5.17677724190782	8.52455236312315
Ga	7.70323649946526	22.19236225762780	7.44702677662214
Ga	3.91146685425269	16.74312905596418	7.48123831096360

Ga	3.75558096592823	11.18411341266495	7.53264723098749
H	4.60139081412213	6.22734722848289	7.60533347030878
Ga	11.49529934427895	16.74328301522980	7.48006896906837
Ga	11.64933104815552	11.18547150858071	7.53282589593417
H	10.80504975095048	6.22734636291882	7.60533301137092
P	5.78419309479870	17.72053359146362	4.00272571346305
P	5.76111435726094	12.29356279148864	3.98073344878516
P	5.79022914759696	6.82529418803596	3.94844085510752
H	6.38704576089974	22.71684340863201	4.00420316747035
H	12.85194064523405	17.25642356139037	3.96807756578038
P	13.48004364515350	12.28758375212622	3.98591779171397
P	5.81535290380435	17.88598173516183	8.10761543011328
P	5.75870377936554	12.34908032152044	7.99714166559487
P	5.76851332283791	6.94484030349355	8.02047128349556
H	6.39778590327004	22.90385781115984	7.89512874862672
H	12.85064301117337	17.45114206754805	7.85597212928565
P	13.54398200859240	12.44480666208855	8.08546558814744
H	7.70321978781886	4.53002826396457	2.61196074367591
H	7.70321995100177	20.84237187614229	2.68056198736731
H	7.70322004171497	15.40326658166121	2.65531110936824
H	7.70321993011592	9.95986315694475	2.62421714976702
H	3.85161003451786	15.39798399997347	2.64793622501820
H	3.85160995230728	9.96381130552740	2.62972781311284
H	11.55483005475303	15.39798438622286	2.64793739855697
H	11.55482991017317	9.96381191760142	2.62972864239404
H	2.55450150283908	17.25642176111137	3.96807763024010
P	1.92636094141910	12.28766003584653	3.98597739764948
P	9.62222149347192	17.72035040945788	4.00248630508357
P	9.64537908226275	12.29358527000847	3.98077957576365
P	9.61604188233012	6.82499151175150	3.94823049183607
H	9.01939430109873	22.71684266647721	4.00420259320216
H	0.63926635576755	14.47657187702958	5.89317720131455
H	14.76717415957145	14.47657321007861	5.89317634453941
P	7.70321338211011	4.09892407536663	6.01073238245391
P	7.70329899790338	20.48134241491946	5.90367515567937
P	7.70313616579889	15.01840432824883	5.88924409950043
P	7.70371294949483	9.51799250112814	5.79751225530461
H	4.48384938321708	19.92840914340503	5.92900068286111
P	3.87233787544794	15.02917326219919	5.89607289688165
P	3.83762792625686	9.52151044365628	5.86209234761318
H	10.92259226392576	19.92841040215319	5.92900143743323
P	11.53436002493276	15.02893141015198	5.89561738841927
P	11.56897114373633	9.52190578007128	5.86239840408940
H	2.55579669664015	17.45114107433681	7.85597166444768
P	1.86226259990580	12.44479506945227	8.08589185229965
P	9.59164557278799	17.88681344480984	8.10530730616717
P	9.64728111272693	12.35239183821393	7.99910603805013
P	9.63794934456249	6.94507221023436	8.02010519322953
H	9.00865299921462	22.90385827893852	7.89512907471426

C	6.46094049944628	16.16710575857597	11.21139896858363
C	6.48031908924847	15.02465271613345	10.42981922288969
C	8.85723983228972	15.03419649138412	10.40532997600025
C	8.88284198833978	16.17659277941570	11.18711868649178
C	7.67376145395500	16.74549704527310	11.59863045521769
H	7.67654966670450	17.63904453824803	12.21145872522853
H	9.83291732501373	16.61187298764725	11.46550361372357
H	9.73093470057646	14.50999130573221	10.04136729229324
H	5.60370370998279	14.49370630187800	10.08339484097162
H	5.51316535954674	16.59476372260941	11.50899931457278
N	7.66715526609029	14.49745277526494	10.06071573283740
H	7.66247236967541	13.63724245519772	9.50609065228085

2) CO₂

Energy=-8454.66683799281

H	5.77741500807466	18.48719899067077	2.80454900748068
H	5.77741501168540	13.04046301999951	2.76832999735591
H	5.77741498704722	7.59242000592054	2.73413699540458
H	13.48063492032984	13.03905306343783	2.77042299448655
H	6.55859679584251	3.22350904693930	5.83627499557434
Ga	5.80309450977920	19.12028889414647	5.98900205538816
Ga	5.77373703574995	13.67493666619973	5.98639236793897
Ga	5.80241230359194	8.11976869175883	6.04316417177556
Ga	13.46314793219535	13.68297510039119	6.03291239680104
H	12.70392598172041	8.66726201523014	5.87242499608394
H	1.92580503969608	13.03905203463420	2.77042498201381
H	9.62902498480214	18.48719899867005	2.80454898708233
H	9.62902499010997	13.04046301836827	2.76833099871827
H	9.62902495305099	7.59242104967203	2.73413495785930
H	0.77682495684306	11.44172596248699	3.92960801188056
H	14.62961407928037	11.44172592555883	3.92960801281740
Ga	7.70307793203827	16.35067160058844	3.87656012366654
Ga	7.70315420800157	10.90699951806080	3.85446218320626
Ga	7.70301376908502	5.31786357234429	3.94493814681218
Ga	7.70319740767763	21.84268288672195	3.88808064255986
Ga	3.82912718057432	16.35824120277004	3.87302009703879
Ga	3.83633393941499	10.87400621960869	3.86663235913470
H	4.62961998301364	5.99564099942780	3.89357699519507
Ga	11.57740047690369	16.35816466076249	3.87315178319311
Ga	11.57058432167222	10.87443885077196	3.86640058275760
H	10.77682104526209	5.99563895240138	3.89357702611528
Ga	1.94341924752347	13.68318877391414	6.03247155244519
H	2.70251297729835	8.66726098260913	5.87242500183839
H	8.84784121520130	3.22350892108456	5.83627600454378
Ga	9.60297176406253	19.12106893347567	5.98766277463074
Ga	9.63258685714206	13.67502618106753	5.98625984391211
Ga	9.60418342470337	8.11970747016474	6.04283978549820
H	0.74840101460530	11.67346300067037	7.64098899965044
H	14.65803996696598	11.67346299959907	7.64099000200815

Ga	7.70372080240676	16.65305433720700	7.54570093954967
Ga	7.70334699468185	11.18180695337323	7.45785961013534
Ga	7.70350759120029	5.17425540930872	8.51866699829771
Ga	7.70328782825287	22.19074435343378	7.44511122967961
Ga	3.91175851662930	16.73203804642415	7.49582202934317
Ga	3.76217373695375	11.18156887843115	7.51975595023377
H	4.60139099118459	6.22734700230655	7.60533299899316
Ga	11.49479889941965	16.73217769106850	7.49557518525058
Ga	11.64403557439611	11.18143116303602	7.51944277246825
H	10.80505000918692	6.22734599403352	7.60533300132711
P	5.78588111446113	17.72103912768467	4.00468725825322
P	5.76190219010529	12.29641564789091	3.98293194884342
P	5.79031800238337	6.82659490012502	3.94963578820690
H	6.38704587362551	22.71684304073728	4.00420302526899
H	12.85194108729049	17.25642405185412	3.96807803783966
P	13.47981566050739	12.28781836973352	3.98638624419262
P	5.81632165024712	17.87861366173876	8.10889749204565
P	5.74309531770448	12.35440543743381	8.00641784094050
P	5.76935689786241	6.94364444089389	8.02037405585304
H	6.39778608648227	22.90385801120807	7.89512899499767
H	12.85064299126452	17.45114199238255	7.85597199447792
P	13.53949174493017	12.43817969712937	8.08286322948674
H	7.70322002691572	4.53002801216904	2.61196102015374
H	7.70322002671164	20.84237191538629	2.68056193008987
H	7.70322000134788	15.40326601792733	2.65531102983118
H	7.70321999222171	9.95986298198194	2.62421700098225
H	3.85161004147772	15.39798395122702	2.64793597893352
H	3.85160999282822	9.96381099690713	2.62972801026135
H	11.55482994144119	15.39798395317126	2.64793696336701
H	11.55483001147444	9.96381197276601	2.62972900416813
H	2.55450093017828	17.25642205319505	3.96807801971828
P	1.92681550191094	12.28757988298693	3.98627371147364
P	9.62064847112132	17.72079127140864	4.00450889703046
P	9.64458448287312	12.29638362442946	3.98288438832525
P	9.61605552352296	6.82639956751319	3.94944568410309
H	9.01939410032377	22.71684305501977	4.00420301886765
H	0.63926597168036	14.47657200475048	5.89317699831898
H	14.76717404634921	14.47657302852066	5.89317599732932
P	7.70319181277834	4.09921919518835	6.00863161921339
P	7.70286201961981	20.47815491135653	5.90496728693685
P	7.70329440131764	15.01676175176755	5.88680702705706
P	7.70318685192076	9.53279120751362	5.81077875580251
H	4.48384901149645	19.92840898295639	5.92900100563514
P	3.87191416108393	15.02951671014013	5.89531247325724
P	3.83787600941072	9.51802058624193	5.85618589058097
H	10.92259298469088	19.92841098690904	5.92900101101321
P	11.53463550195758	15.02938037273854	5.89554310893424
P	11.56863937750931	9.51808186367281	5.85579557814688
H	2.55579701630218	17.45114098507168	7.85597199348538

P	1.86670322390388	12.43859352626378	8.08269467558359
P	9.59054168816689	17.87938124890392	8.10828675844100
P	9.66333852631871	12.35434232547479	8.00637118877783
P	9.63714999325144	6.94383698702404	8.02035190196876
H	9.00865291593616	22.90385797919369	7.89512899445096
O	7.70824902115629	14.85831711494767	9.68123962698629
O	7.70741402925478	12.86653443102144	10.90729063111471
C	7.71099031184256	13.85058945719871	10.27853745368031

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Energy=-8455.87033163748

H	-1.90788300549772	5.27555299372941	-3.13827099602762
H	-1.90204601140109	-0.17109699833802	-3.18737401296873
H	-1.89620395961896	-5.61905996513374	-3.23445400096373
H	5.80117895743443	-0.16416295305961	-3.19961802270052
H	-1.10451502494594	-9.99446100591201	-0.14410400105484
Ga	-1.87656508715233	5.90363255143487	0.04209643631589
Ga	-1.89216571972669	0.44617922519116	0.03017762930861
Ga	-1.84356714087100	-5.08970146554527	0.08131249925298
Ga	5.78750901112767	0.47343816803205	0.06371351333419
H	5.03498200374182	-4.54413300790684	-0.10651200446233
H	-5.75365100572604	-0.17668799627551	-3.17811600635795
H	1.94372700055903	5.27972799685957	-3.14543799827440
H	1.94956398454700	-0.16692300700876	-3.19454000825024
H	1.95540594269700	-5.61488393421702	-3.24162304258369
H	-6.89874300011290	-1.77800200595859	-2.02057299876720
H	6.95404704052545	-1.76298605252809	-2.04634898023482
Ga	0.02276815823928	3.13563470497186	-2.07220400273464
Ga	0.03381586329233	-2.31377595783426	-2.10230314476242
Ga	0.03768259471576	-7.88923462737075	-2.03283693422491
Ga	0.01634370659703	8.63101668662548	-2.05090500911245
Ga	-3.85238102145735	3.13931974352874	-2.06875201255748
Ga	-3.83687409761162	-2.34428145633365	-2.08861632280874
H	-3.04011105021081	-7.21982503651092	-2.07665499098651
Ga	3.89774346426766	3.14724856576897	-2.08309131158329
Ga	3.89245879371246	-2.33643734842290	-2.10046771089703
H	3.10709006980617	-7.21316406440810	-2.08809397155731
Ga	-5.72910431408204	0.46250452939332	0.08296151814830
H	-4.96643200155159	-4.55497399645186	-0.08790100199512
H	1.18472901669852	-9.99197999779586	-0.14836199933618
Ga	1.92373780139656	5.90649810274677	0.03574087599100
Ga	1.95642263323260	0.44104345673844	0.03521405139549
Ga	1.92396514736806	-5.08177809396625	0.08642726650733
H	-6.92051200555744	-1.55507400068070	1.69140899378216
H	6.98912697457252	-1.53999699110168	1.66552800255994
Ga	0.02894243023948	3.44653122666349	1.58210953989214
Ga	0.06094311909189	-2.14427994315426	1.63763316172980
Ga	0.05483882157547	-8.02191335700683	2.54245501232083
Ga	0.02257036930389	8.97005892584142	1.50722120080776

Ga	-3.76286668826425	3.50641969416154	1.54858627437684
Ga	-3.90977110290874	-2.03433927515908	1.55187188592365
H	-3.06168500207941	-6.99692899831637	1.63570200276691
Ga	3.82268598935879	3.51122376635064	1.53049983639385
Ga	3.97120679682410	-2.02169265030646	1.56160046788169
H	3.14197400369580	-6.99020599854687	1.62415800332605
P	-1.89634015939873	4.50514322292364	-1.94071424422169
P	-1.91065344097705	-0.92434302392674	-1.97656647632616
P	-1.88058323654542	-6.38523310202450	-2.01821524972594
H	-1.30060399871360	9.50302000234008	-1.92974800146376
H	5.17014199370384	4.04969400016775	-1.99081799626004
P	5.80237007509714	-0.91964661157884	-1.98552498344198
P	-1.86041486644571	4.65842692253791	2.16101403249372
P	-1.91938585820836	-0.88022080857205	2.04384898949391
P	-1.89685758708590	-6.27531182406083	2.05476992654441
H	-1.28282700216795	9.68084400289631	1.96160099783383
H	5.17586800030336	4.23521500087063	1.89753900227548
P	5.87568510095898	-0.77264501574470	2.11357874890450
H	0.03269300230125	-8.67907501042859	-3.36745698869700
H	0.01513899723558	7.63310699979033	-3.26027199797580
H	0.02098699888814	2.19405999517985	-3.29838700571180
H	0.02683000915534	-3.24926895477504	-3.34235695378361
H	-3.83063100826978	2.18462101315710	-3.29860799011912
H	-3.82477400485046	-3.24950900534397	-3.32967001400679
H	3.87258900193831	2.19297099855034	-3.31294100066052
H	3.87844601144916	-3.24115800850020	-3.34400300026707
H	-5.12729698929890	4.03852998918601	-1.97165700503909
P	-5.74875018781048	-0.93207337101613	-1.96434427232484
P	1.93907238639514	4.50931266917262	-1.94792108034021
P	1.96754835391206	-0.91562587681842	-1.98242159065398
P	1.94875367224527	-6.37748284750590	-2.02133728432564
H	1.33174299823139	9.50587299733030	-1.93464600189935
H	-7.03593695982748	1.25205098593276	-0.04956998826859
H	7.09197100750059	1.26736499799716	-0.07585999591974
P	0.03978952698258	-9.11663759745462	0.02928002613920
P	0.02220500455842	7.26229773046180	-0.03816424829997
P	0.03095577544395	1.79406905389395	-0.06279112457394
P	0.03761855357845	-3.65864288242553	-0.15491592802356
H	-3.19719600434137	6.70797000055302	-0.00800500181253
P	-3.79802169428113	1.80341275211054	-0.05194862230191
P	-3.82833411929364	-3.70608895630107	-0.10215501727445
H	3.24154700221030	6.71495099971788	-0.01998500042541
P	3.85429945109300	1.81165286228459	-0.07053256831846
P	3.89926257996961	-3.68969909809599	-0.10887039188502
H	-5.11897799581335	4.22405399412940	1.91669499346331
P	-5.80308661317440	-0.78841008624259	2.13201205826117
P	1.92001726328424	4.65980107851120	2.15291915480184
P	1.99360900631908	-0.84997994025424	2.05119016579378
P	1.99194657542900	-6.26050202457563	2.06461360134343

H	1.32803999755819	9.68367399985690	1.95674199742160
O	-1.74284040750306	-3.24125276721763	4.42698235527013
O	0.14158841565502	-3.56620769546638	3.20349134881361
C	-0.67657679909503	-3.91781572238004	4.06255288072998
H	-1.81104753711359	-2.39400935183209	3.92715796850969
H	-0.53613978854222	-4.83493332953302	4.63339494563488

4) H₂O

Energy=-8342.59172690791

H	5.77741514427930	18.48719919049401	2.80454892259286
H	5.77741502176823	13.04046333390572	2.76833018551478
H	5.77741493058181	7.59242012118861	2.73413664634603
H	13.48063505651977	13.03905262120290	2.77042346825879
H	6.55859737253350	3.22350851319041	5.83627545828471
Ga	5.80260674420405	19.10066763850211	6.01476936957180
Ga	5.78909053534936	13.69010112277059	5.95905904875956
Ga	5.80307190312442	8.12306038525882	6.04694645056598
Ga	13.46093740016325	13.68659716418492	6.02848552245376
H	12.70392630438919	8.66726173731988	5.87242506364813
H	1.92580496184028	13.03905178471078	2.77042467056195
H	9.62902515155943	18.48719934258668	2.80454882682063
H	9.62902499063174	13.04046304373167	2.76833073608290
H	9.62902477909587	7.59242111956160	2.73413532996225
H	0.77682473311774	11.44172606054793	3.92960752659410
H	14.62961391650445	11.44172599179871	3.92960799930573
Ga	7.70327832903852	16.35854952952631	3.87199456191545
Ga	7.70294150201267	10.90816053966712	3.85331625102929
Ga	7.70244454351131	5.31796511176125	3.94603357719559
Ga	7.70319456925623	21.83530617368483	3.89727497094216
Ga	3.83292129604200	16.36110205833524	3.87349579059572
Ga	3.83337482378217	10.87193363641741	3.86840604545672
H	4.62962024463570	5.99564053865117	3.89357732867221
Ga	11.57359840158065	16.36103186572652	3.87357351601902
Ga	11.57292895524403	10.87203927245234	3.86820155289646
H	10.77682065787722	5.99563911199062	3.89357710788047
Ga	1.94574745726767	13.68702271523590	6.02886192052601
H	2.70251345925222	8.66726133219125	5.87242542389615
H	8.84784133833131	3.22350893884956	5.83627574365438
Ga	9.60379900928727	19.10059484776649	6.01483172437295
Ga	9.61749173112566	13.69014118701345	5.95875348776473
Ga	9.60430141828130	8.12329756040615	6.04575389217919
H	0.74840070232735	11.67346252074895	7.64098898638267
H	14.65803970522537	11.67346263782713	7.64098962615750
Ga	7.70332351609056	16.52032371172086	7.69465050415296
Ga	7.70340811728880	11.19288236610823	7.46512131521416
Ga	7.70691567748169	5.17209081353155	8.52180554893805
Ga	7.70323725506420	22.18482887299611	7.44636553903912
Ga	3.91256966346715	16.72742381438302	7.50528003066626
Ga	3.75758007260321	11.20060060643588	7.53007001228157

H	4.60139072046671	6.22734720334565	7.60533345033113
Ga	11.49398953844113	16.72706179767837	7.50523292314255
Ga	11.64883190057724	11.20107263560666	7.53066055949331
H	10.80504979810620	6.22734635300688	7.60533299611823
P	5.78613035306086	17.72426633631002	4.00672352303904
P	5.76023913274071	12.29193123857201	3.97909543740274
P	5.78967124296900	6.82864746077423	3.95116501843159
H	6.38704564126020	22.71684344648981	4.00420319584558
H	12.85194062368843	17.25642355338767	3.96807755321133
P	13.48029047959028	12.28765877155723	3.98613217688940
P	5.82268953643892	17.85214359474725	8.11697241546529
P	5.75178315761903	12.37938583230299	8.00083739599586
P	5.76920224554996	6.94309815725553	8.02044562593514
H	6.39778582122909	22.90385778227065	7.89512878525617
H	12.85064299028609	17.45114198250768	7.85597217261342
P	13.54801489994022	12.44971352504189	8.08563220246336
H	7.70321978911506	4.53002825572565	2.61196080710880
H	7.70321993789413	20.84237172108263	2.68056186835565
H	7.70322002372422	15.40326647535822	2.65531103294299
H	7.70321993292782	9.95986319015093	2.62421714765978
H	3.85161002672522	15.39798402353429	2.64793619589826
H	3.85160994914949	9.96381130174088	2.62972780836353
H	11.55483005864852	15.39798438649643	2.64793740730077
H	11.55482991851437	9.96381190444030	2.62972863837498
H	2.55450154106411	17.25642173980221	3.96807764203249
P	1.92610126635195	12.28773858474170	3.98620493191240
P	9.62037918796276	17.72426079062917	4.00673809283191
P	9.64604278284509	12.29178486601545	3.97901307445720
P	9.61665908633893	6.82822291294132	3.95072914542871
H	9.01939444758743	22.71684273374330	4.00420262916837
H	0.63926638531409	14.47657186729677	5.89317720669912
H	14.76717412033501	14.47657320113052	5.89317634564342
P	7.70314939983987	4.09891155849114	6.00905330745969
P	7.70325467583532	20.46571475533318	5.91376979254959
P	7.70323862373696	15.04311484342086	5.86645217751018
P	7.70342609436794	9.54123787606614	5.81789538352997
H	4.48384897892522	19.92840931540783	5.92900069975109
P	3.87331495926576	15.02880530678528	5.89499564026743
P	3.83700166042190	9.52558648696861	5.86571725991575
H	10.92259267964357	19.92841065978814	5.92900140504221
P	11.53333268144752	15.02852378240670	5.89500992507337
P	11.56975327462173	9.52607827537405	5.86594546879956
H	2.55579667846545	17.45114107835720	7.85597168648766
P	1.85855851608943	12.44947711057521	8.08565533458561
P	9.58392897392811	17.85205744685273	8.11692367116512
P	9.65457000481417	12.37972602230377	8.00107114939859
P	9.63706193265669	6.94361879318094	8.01989092894420
H	9.00865308373333	22.90385829129503	7.89512908558599
O	7.70326473072300	14.97192527714834	9.25022145078191

H	8.47517475765272	14.37213344153829	9.17044917848725
H	6.92999314270636	14.37357700516109	9.17184887886621

5) o-DHP

Energy=-8515.51957769954

H	5.77741511032167	18.48719912998668	2.80454891125823
H	5.77741498418311	13.04046331152917	2.76833019260381
H	5.77741486233964	7.59242003517445	2.73413669613099
H	13.48063510444653	13.03905259943055	2.77042344674134
H	6.55859713261577	3.22350859042331	5.83627544680194
Ga	5.80192987417227	19.11884062894635	5.98324615120095
Ga	5.78545615289018	13.65134920084218	5.98775410778848
Ga	5.82485686391743	8.13339870087365	6.03366530533005
Ga	13.45692992355193	13.69059187083506	6.02598848120665
H	12.70392634213548	8.66726177048132	5.87242505619644
H	1.92580492734185	13.03905178439587	2.77042461753761
H	9.62902514965795	18.48719928412056	2.80454878927492
H	9.62902501752499	13.04046301045468	2.76833077409375
H	9.62902495810811	7.59242094541517	2.73413537965538
H	0.77682478682723	11.44172606931095	3.92960753710935
H	14.62961387529250	11.44172602216532	3.92960799846810
Ga	7.70369222288537	16.34747416508850	3.87934625085518
Ga	7.70259484179810	10.89310866947736	3.87365441611505
Ga	7.70440058384960	5.32551529641429	3.94236571199226
Ga	7.70327905682917	21.84213614366560	3.88864049578672
Ga	3.82682114574910	16.35283918579155	3.87792967301050
Ga	3.84471589752028	10.86790755689111	3.87619990215909
H	4.62962031990430	5.99564060916088	3.89357730520626
Ga	11.57759199038731	16.35596163771521	3.87547865782926
Ga	11.56435049533259	10.87038205040562	3.87246362949587
H	10.77682041140681	5.99563930143893	3.89357705693346
Ga	1.94416950733371	13.68095812022806	6.03175314646760
H	2.70251341495350	8.66726129441810	5.87242542691522
H	8.84784161974880	3.22350880880585	5.83627574323452
Ga	9.60370236703335	19.12022976017774	5.98367038248314
Ga	9.62371777992002	13.65066458733989	5.98686098362322
Ga	9.58024977854462	8.14044376715341	6.04291414455803
H	0.74235906138380	11.64697401650587	7.64093317077907
H	14.65193821065563	11.67486488873692	7.61113872653770
Ga	7.70365772740278	16.66149012879677	7.52536289567962
Ga	7.69316302926590	11.07864051758238	7.69708941463133
Ga	7.71221805459276	5.14953720150697	8.49340981199274
Ga	7.70320180460177	22.18895848031972	7.44544448154661
Ga	3.90810917406330	16.72255543314703	7.48561909329590
Ga	3.78381954353636	11.21193584486218	7.53382787283398
H	4.60139073592529	6.22734719484036	7.60533345368542
Ga	11.49656523101867	16.72655180074632	7.48642548279825
Ga	11.63049354006105	11.21167264214463	7.51785548777073
H	10.80504973648916	6.22734639643455	7.60533303546714

P	5.78482560501712	17.71833697539354	4.00294985694210
P	5.76605051394368	12.29194438618827	3.97934425999589
P	5.78998228916524	6.83002027712766	3.94928654852269
H	6.38704567649561	22.71684346254662	4.00420319943011
H	12.85194058291688	17.25642350764042	3.96807755074515
P	13.47775031004586	12.28576679316482	3.98603087097153
P	5.81216074577986	17.87409962993596	8.10248056462258
P	5.74714034365038	12.39767017658975	8.01057775185124
P	5.79849834238497	6.90590909208642	7.98290475249471
H	6.39778579143078	22.90385777846653	7.89512878990586
H	12.85064303351098	17.45114199159382	7.85597218151736
P	13.54459165404955	12.44135310636346	8.07438446066115
H	7.70321981951392	4.53002829120990	2.61196076494104
H	7.70321990839487	20.84237168780210	2.68056182496872
H	7.70322005858776	15.40326655169943	2.65531099463609
H	7.70321994207905	9.95986319976000	2.62421711402511
H	3.85161003477004	15.39798401903949	2.64793616885885
H	3.85160995483102	9.96381134494029	2.62972782737533
H	11.55483007160912	15.39798444278345	2.64793743507444
H	11.55482988725813	9.96381192631273	2.62972865807257
H	2.55450154622942	17.25642175031146	3.96807765751721
P	1.92965641397172	12.28403784069345	3.98585818446270
P	9.62082250974071	17.71986008673714	4.00295834990770
P	9.64101750249641	12.29068988967086	3.97888022244920
P	9.61723849494801	6.83211075995511	3.95265552266262
H	9.01939445759732	22.71684276343378	4.00420264288210
H	0.63926645655462	14.47657186383588	5.89317723878762
H	14.76717411438858	14.47657320693787	5.89317633936947
P	7.70403829939189	4.09936455517092	6.00299039137752
P	7.70262730971629	20.47714263778522	5.90432803052456
P	7.70477922321847	15.01077863273805	5.88252179398990
P	7.69983626078612	9.58250719899895	5.85165714416685
H	4.48384896959121	19.92840928401884	5.92900073690320
P	3.87810269471936	15.01870204537444	5.88953057690580
P	3.84204235424493	9.52013501509795	5.87652616301402
H	10.92259263894727	19.92841060647660	5.92900142477635
P	11.52424581504221	15.02487574223919	5.88816503240899
P	11.56621381135445	9.52053094592811	5.86862191222875
H	2.55579664563354	17.45114111851930	7.85597169468983
P	1.85254437737159	12.42712298348824	8.08058107111185
P	9.59284767343016	17.87708666620986	8.10423934442642
P	9.65958480939737	12.37857094994052	8.00626171361472
P	9.62566027880509	6.93341746867621	8.00805737225802
H	9.00865310927059	22.90385830806031	7.89512909736806
C	6.21819209415216	10.68812076343453	11.05435086308713
C	6.37320894502423	9.77125801217375	10.08698242742745
C	8.80275439663954	9.88394646825712	10.31843318031207
C	8.59658379137588	11.16667978742029	11.08514227060331
C	7.35171220394481	11.52286476243667	11.44981276808345

H	7.16841515187133	12.41507497368377	12.04070621643176
H	9.47003970764129	11.74100465658649	11.37232429580198
H	8.88513852927766	9.02801731283083	11.00517240098819
H	5.59587166170186	9.13215343411413	9.68652430879927
H	5.24776280440794	10.82801574894961	11.51692370226854
N	7.64291101321935	9.66552120473910	9.40450874080575
H	7.72545561075883	8.73502169883040	8.98760716716676
H	9.70687221343080	9.90702098475611	9.70858672005105

6) Py

Energy=-8514.34736214862

H	5.77741512804948	18.48719924432921	2.80454890615459
H	5.77741500245702	13.04046336310690	2.76833019926914
H	5.77741487637974	7.59242006714613	2.73413666930263
H	13.48063504297262	13.03905262717471	2.77042344732262
H	6.55859746597124	3.22350847760179	5.83627543521762
Ga	5.80357653831904	19.10735605710543	5.99668441772911
Ga	5.79848772815791	13.68909778204899	5.99591187309548
Ga	5.80511297531340	8.12230770678216	6.04278200744749
Ga	13.45796305749388	13.68860840103432	6.03437426496642
H	12.70392629749929	8.66726174067618	5.87242506632937
H	1.92580497302964	13.03905179573620	2.77042465410800
H	9.62902517332603	18.48719935999628	2.80454878388093
H	9.62902501397332	13.04046305603816	2.76833074630937
H	9.62902488893663	7.59242104588729	2.73413534981482
H	0.77682473490553	11.44172605455041	3.92960753111487
H	14.62961392249360	11.44172598489900	3.92960800604196
Ga	7.70320887432041	16.33829630876947	3.89778774463855
Ga	7.70305827790276	10.91133035103107	3.85362912342617
Ga	7.70228666033822	5.31882792710859	3.94427236966411
Ga	7.70319615191116	21.83779153686326	3.89455901781625
Ga	3.83444984878489	16.35912897215759	3.87719882583147
Ga	3.84272897642996	10.87738620432551	3.86647588259891
H	4.62962033573370	5.99564060162170	3.89357731117320
Ga	11.57204642708989	16.35907016841351	3.87727287203836
Ga	11.56391902752987	10.87773438561569	3.86603113798962
H	10.77682052699582	5.99563921416260	3.89357710063362
Ga	1.94851055183386	13.68873645007955	6.03449547177810
H	2.70251344909576	8.66726132611625	5.87242542434855
H	8.84784124991610	3.22350896385807	5.83627574328877
Ga	9.60286402813848	19.10722277088427	5.99668772566016
Ga	9.60803178464563	13.68934050540439	5.99556203133777
Ga	9.60263565117573	8.12262321899024	6.04107127605275
H	0.74840071732035	11.67346252177783	7.64098898465090
H	14.65803967604806	11.67346264485413	7.64098962580721
Ga	7.70319079303857	16.55664550745415	7.76674554577241
Ga	7.70352811361494	11.18839828658007	7.45590048563089
Ga	7.70843028538519	5.17660131157004	8.51531826891774
Ga	7.70324091133629	22.18611600718730	7.44221335297312

Ga	3.91875466465421	16.74864944401881	7.49136323066967
Ga	3.77367395575736	11.18816108559175	7.50486875471007
H	4.60139081020368	6.22734722588295	7.60533346837898
Ga	11.48767102107867	16.74842428077441	7.49164790128111
Ga	11.63272933913478	11.18832023805276	7.50522471702110
H	10.80504973900021	6.22734635669616	7.60533301224388
P	5.78930623196855	17.72036283114107	4.00446483646260
P	5.76444979521288	12.30398557259257	3.98772030496054
P	5.79046725463816	6.82659178948960	3.94978020904438
H	6.38704560841949	22.71684347687245	4.00420320384036
H	12.85194065564589	17.25642359943161	3.96807759585156
P	13.47876083487845	12.28800247321341	3.98692098497002
P	5.81091168905929	17.89961215609165	8.09902369793077
P	5.74458350647921	12.35198557212664	8.01057998062212
P	5.76888245966742	6.94346395894058	8.01908019125738
H	6.39778590345754	22.90385780091527	7.89512876676095
H	12.85064304467270	17.45114207847698	7.85597215520110
P	13.53478492670597	12.43458764620005	8.07873771526883
H	7.70321975944415	4.53002822618274	2.61196076853459
H	7.70321995120496	20.84237171147744	2.68056185675251
H	7.70322003292079	15.40326647470290	2.65531102930444
H	7.70321992878430	9.95986314485109	2.62421714576771
H	3.85161005812483	15.39798397268300	2.64793620241137
H	3.85160995075091	9.96381130619502	2.62972782768510
H	11.55483003616838	15.39798434247606	2.64793736607114
H	11.55482991339924	9.96381191030834	2.62972864929935
H	2.55450148049836	17.25642178487455	3.96807764579825
P	1.92780349425240	12.28790573631872	3.98693351595516
P	9.61714844420168	17.72032082379816	4.00443768899626
P	9.64191274209189	12.30391976498974	3.98760952401609
P	9.61598869405284	6.82606654947454	3.94892183865820
H	9.01939446236818	22.71684275561287	4.00420263728493
H	0.63926637083234	14.47657187623129	5.89317720258018
H	14.76717414090521	14.47657320558201	5.89317634503870
P	7.70308614628876	4.09834425013978	6.00706089309014
P	7.70327020928376	20.47235759198865	5.90558659937667
P	7.70316993404968	15.06165917315271	5.92711957628036
P	7.70351759724933	9.53225834966772	5.80894361442546
H	4.48384918285735	19.92840920759073	5.92900071195325
P	3.87908240330531	15.02940954850078	5.90344984502610
P	3.83846980136256	9.51606901792116	5.85219754655533
H	10.92259246032960	19.92841047590055	5.92900145783867
P	11.52747214665587	15.02939218928035	5.90345455588363
P	11.56839542699772	9.51651148661849	5.85209563803395
H	2.55579665414606	17.45114109589542	7.85597168313885
P	1.87174786009169	12.43449336365228	8.07878622855367
P	9.59549116349661	17.89948940725450	8.09912372975249
P	9.66198618689704	12.35248143603815	8.01072431468606
P	9.63767516321001	6.94466004937676	8.01861338571176

H	9.00865299803615	22.90385827790040	7.89512907802791
C	8.90492521373880	14.16180010641041	11.24307875104083
C	8.86303582009828	14.93064606270234	10.08685233987276
C	6.54195787556299	14.93112981653329	10.08653247747031
C	6.49941457462759	14.16244649450091	11.24286460299819
C	7.70200577372721	13.77339199148830	11.83440832449096
H	7.70175730583288	13.17438519496623	12.73864025313306
H	5.54357067838867	13.86897920362749	11.65992864066199
H	5.63817396984597	15.26405232182158	9.59133139603532
H	9.76706968554309	15.26328913994446	9.59189981224852
H	9.86055416624190	13.86790047493095	11.66032012520069
N	7.70264390181830	15.32144694053845	9.52484713085970

7) HCOO⁻

Energy=-8455.4268180488

H	5.77741497316535	18.48719902446741	2.80454898504156
H	5.77741496307586	13.04046300617294	2.76832999055208
H	5.77741494897780	7.59241992612725	2.73413703286902
H	13.48063513198204	13.03905290653985	2.77042304378111
H	6.55859694352072	3.22350906684411	5.83627502558641
Ga	5.80188664014282	19.11701424465183	5.97922183210379
Ga	5.76326334696136	13.72213787281303	5.91265324763358
Ga	5.79717073620334	8.13924072755641	6.06199824171970
Ga	13.45689329063524	13.68292608744128	6.03555109201342
H	12.70392594911378	8.66726200139769	5.87242503376456
H	1.92580491434490	13.03905191877387	2.77042505574988
H	9.62902500209183	18.48719900347178	2.80454902696505
H	9.62902501374810	13.04046301423248	2.76833098150544
H	9.62902495224214	7.59242098941894	2.73413498905806
H	0.77682509227916	11.44172608800593	3.92960794043384
H	14.62961385913186	11.44172613055770	3.92960796607553
Ga	7.72042139901982	16.35790436228976	3.87012975354020
Ga	7.69386298150500	10.88943900583866	3.88136035909868
Ga	7.69985493692022	5.33620593832214	3.94003483294961
Ga	7.70333497545529	21.84105592077821	3.89002070191621
Ga	3.82367377251672	16.36259933959256	3.86705328948992
Ga	3.83963639093007	10.85180267534735	3.89929025241588
H	4.62962003492774	5.99564105970041	3.89357698699080
Ga	11.57805934454501	16.34217575648551	3.88956255180075
Ga	11.55423107048042	10.86845277195968	3.87862281177568
H	10.77682102346139	5.99563899219504	3.89357701844383
Ga	1.94656141693479	13.65554681104624	6.07157210726492
H	2.70251304962921	8.66726101696507	5.87242497762271
H	8.84784106467107	3.22350897507293	5.83627601976284
Ga	9.60442876567110	19.11883144630864	5.98729044528142
Ga	9.59130859419535	13.61899750738095	6.03716761857351
Ga	9.55587382702649	8.15669754037698	6.07506214998236
H	0.74840097740692	11.67346298159937	7.64098900411521
H	14.65804008127296	11.67346297869709	7.64098998980358

Ga	7.69854369058100	16.66172354364554	7.51453530957797
Ga	7.52090408485707	11.10892446755087	7.68946815170371
Ga	7.70459119450742	5.14787236153349	8.47360319877459
Ga	7.70311379117496	22.18871595936293	7.44404718364431
Ga	3.90726208003752	16.72572892534127	7.46997289575269
Ga	3.91385292960919	11.11880332321823	7.72659015892463
H	4.60139080102443	6.22734694280266	7.60533295754174
Ga	11.49575816642339	16.71999259744690	7.48828430362901
Ga	11.60565873489875	11.18602760145756	7.55115348684280
H	10.80505020461314	6.22734593959865	7.60533298020173
P	5.78909344361153	17.71647290863169	3.99957386269077
P	5.75871511951595	12.29223549809202	3.97324719114001
P	5.78608209912338	6.83688977599565	3.95706093115599
H	6.38704602907423	22.71684297997705	4.00420298713459
H	12.85194101773425	17.25642400558240	3.96807796474955
P	13.47469211384067	12.28317530772553	3.98635358941093
P	5.80995050638591	17.87634436942776	8.10030996244222
P	5.73164209726017	12.60349425255101	7.93370930656319
P	5.81046991816409	6.87406551851769	7.99320445631385
H	6.39778618856335	22.90385801568269	7.89512894619733
H	12.85064291379156	17.45114198297257	7.85597197138775
P	13.53321300749997	12.43377680917723	8.08150668238125
H	7.70322003326066	4.53002805546192	2.61196101718449
H	7.70322005879567	20.84237209958337	2.68056210314024
H	7.70322000096474	15.40326602724817	2.65531102197586
H	7.70322001375128	9.95986298924287	2.62421696879877
H	3.85160999324185	15.39798401622299	2.64793604437456
H	3.85161000862268	9.96381104277500	2.62972807447515
H	11.55482999626921	15.39798401774550	2.64793703294170
H	11.55482999962872	9.96381202741628	2.62972899923314
H	2.55450099688804	17.25642199693420	3.96807797442403
P	1.93074897377764	12.28493801162919	3.99050043873836
P	9.62964062393782	17.72428279073700	4.00263825676157
P	9.63368979816345	12.29136909923115	3.98627382706065
P	9.61759817653102	6.83943553911568	3.96047381793748
H	9.01939388153176	22.71684293248502	4.00420297110970
H	0.63926600743774	14.47657202139339	5.89317697201999
H	14.76717389879949	14.47657295265338	5.89317600001054
P	7.70479006021374	4.10091639459743	5.99730604830532
P	7.70293584428561	20.47686025885401	5.90393575693525
P	7.71231519273897	15.03213277861537	5.85763924139073
P	7.66839793360833	9.59076289197149	5.86356698283270
H	4.48384906344510	19.92840897247742	5.92900099597791
P	3.84569502047769	15.04858748332772	5.85876977053678
P	3.83841652126333	9.54033213306747	5.90201373404423
H	10.92259297906380	19.92841099819426	5.92900099604180
P	11.50778331737285	14.99901559664385	5.90693192589029
P	11.56058831159378	9.51599882866486	5.87449925683434
H	2.55579807707185	17.45114096621418	7.85597197073159

P	1.90303237832830	12.39089808122212	8.09016971739885
P	9.59105280577440	17.87406792410626	8.10408857813855
P	9.59540488385358	12.30053992410592	8.05904064059859
P	9.62197731248699	6.92169225298887	8.01992205998100
H	9.00865282276800	22.90385794177774	7.89512896726204
O	4.58377871340111	9.91325068773136	9.28232622718401
O	6.89062170235409	9.87330403003188	9.23271177875533
C	5.74103180019812	9.55011971336127	9.67403745551267
H	5.74955196630551	8.90358132124207	10.56028195225083

8) OH⁻

Energy=-8342.11649408864

H	5.77741516684023	18.48719922956843	2.80454893531904
H	5.77741504405104	13.04046334277403	2.76833019459369
H	5.77741497700976	7.59242012756929	2.73413664263735
H	13.48063502141475	13.03905264238155	2.77042344769195
H	6.55859716780291	3.22350855963149	5.83627548204765
Ga	5.80811829758472	19.10101549098711	6.01067978881045
Ga	5.81409118192654	13.71915203004064	5.98712082532613
Ga	5.80198547386638	8.12675146240747	6.04476046414851
Ga	13.45142845238888	13.69771243706812	6.03502433549750
H	12.70392633975050	8.66726170639960	5.87242507059072
H	1.92580501029361	13.03905178455481	2.77042464454398
H	9.62902513925677	18.48719936846803	2.80454884593617
H	9.62902498727722	13.04046306591080	2.76833076460170
H	9.62902487176604	7.59242101722981	2.73413532681690
H	0.77682473576545	11.44172605307509	3.92960755738607
H	14.62961392911736	11.44172597743246	3.92960801760052
Ga	7.70330171117407	16.33910852742334	3.90377777139060
Ga	7.70365517866706	10.91684096291459	3.85075839908766
Ga	7.70342112401337	5.32110052117021	3.94412771952201
Ga	7.70320970739688	21.83553351789838	3.89752373362568
Ga	3.83787633580141	16.35880597314366	3.88316113697525
Ga	3.84495270247854	10.88067140432396	3.86607219543692
H	4.62962017529591	5.99564049236915	3.89357735118584
Ga	11.56865764859091	16.35867551212788	3.88326214634050
Ga	11.56204253170270	10.88095322368055	3.86574287105406
H	10.77682050581114	5.99563922565873	3.89357711189646
Ga	1.95508664327103	13.69793324798946	6.03488315201286
H	2.70251336572305	8.66726123785625	5.87242541152112
H	8.84784156404108	3.22350884778785	5.83627574404195
Ga	9.59839272287718	19.10083049799851	6.01081438521137
Ga	9.59251473862672	13.71929100700610	5.98736051596217
Ga	9.60573066095037	8.12658074474024	6.04415924691572
H	0.74840075600780	11.67346254711187	7.64098899853855
H	14.65803966628963	11.67346265554421	7.64098963593783
Ga	7.70340086962116	16.46567560782293	7.92567759829207
Ga	7.70363418493119	11.18845356087126	7.45746254159209
Ga	7.70276307065925	5.17140334728380	8.51403526568179

Ga	7.70322816792144	22.18384481834235	7.43930030722563
Ga	3.93635251929880	16.75670187804036	7.51956583937755
Ga	3.77579417009635	11.20156638921892	7.51676001618593
H	4.60139081084652	6.22734724629134	7.60533348108175
Ga	11.47009218461838	16.75660786387140	7.51962458100778
Ga	11.63074418901237	11.20154282915008	7.51730228941360
H	10.80504975220541	6.22734637552285	7.60533303500539
P	5.79033220863345	17.72368918497911	4.00625450315198
P	5.76516957757140	12.30847017259738	3.99096886825115
P	5.78948058037835	6.82853746934943	3.95035209493268
H	6.38704562639483	22.71684344617440	4.00420320394123
H	12.85194071349209	17.25642366518589	3.96807763885613
P	13.47890979264442	12.28935793390383	3.98834349267844
P	5.82996980404166	17.91011401953277	8.10197302704064
P	5.75677080662142	12.37179934328646	8.01041631304128
P	5.77214469153874	6.94100798834970	8.01722577597724
H	6.39778593916146	22.90385778816255	7.89512876129248
H	12.85064295712598	17.45114196415445	7.85597216391883
P	13.53954480243630	12.44123417201853	8.08085826549105
H	7.70321983638230	4.53002827509958	2.61196067933998
H	7.70321997369804	20.84237172865003	2.68056189093773
H	7.70322001732025	15.40326643254070	2.65531105203865
H	7.70321992424355	9.95986316871646	2.62421716236844
H	3.85161004240331	15.39798398426653	2.64793618957246
H	3.85160993739932	9.96381134572238	2.62972782562620
H	11.55482999887934	15.39798425468285	2.64793730053791
H	11.55482991730648	9.96381185843936	2.62972858418249
H	2.55450151113051	17.25642176884911	3.96807764939804
P	1.92767407668401	12.28919334952415	3.98828284756155
P	9.61621313324460	17.72368308395003	4.00625348026366
P	9.64168789129464	12.30862060311212	3.99105091770287
P	9.61682555679510	6.82845689546878	3.95049489732099
H	9.01939442193980	22.71684272125469	4.00420262736560
H	0.63926624652893	14.47657190526924	5.89317720591425
H	14.76717421350486	14.47657325127248	5.89317635264097
P	7.70314222567991	4.09967390612857	6.00753014486145
P	7.70328784943699	20.47514695103414	5.90081028516072
P	7.70326943629708	15.10236997050198	5.94660622968660
P	7.70380072737618	9.53690225645352	5.80918959334266
H	4.48384888398382	19.92840936894543	5.92900069929549
P	3.88107311763744	15.04009551715913	5.91271998933203
P	3.83753411386962	9.52295720273249	5.85809386196054
H	10.92259271452265	19.92841067619020	5.92900140845343
P	11.52550070338540	15.04011745424098	5.91278970353003
P	11.56948496773928	9.52363484524926	5.85804386899114
H	2.55579677343861	17.45114104614019	7.85597165852462
P	1.86697170438895	12.44124835646180	8.08058236912080
P	9.57656159231940	17.91027730102587	8.10220106089096
P	9.64992786138208	12.37214120715931	8.01075837119183

P	9.63465676776925	6.94133354717620	8.01759029935888
H	9.00865297126839	22.90385825400208	7.89512907310303
O	7.70340684394831	15.29446496494515	9.43248581677266
H	7.70536811771052	14.37248599702844	9.13353158507945

9) H₂O + H⁺

Energy=-8343.05392020489

H	5.77741506237040	18.48719917845306	2.80454899031619
H	5.77741494035755	13.04046327789617	2.76833029765026
H	5.77741496428478	7.59242013037304	2.73413665299245
H	13.48063515802908	13.03905254574339	2.77042347300364
H	6.55859725823773	3.22350839716749	5.83627544317922
Ga	5.80577025022970	19.12971555941600	5.98115282464106
Ga	5.79443196270176	13.69750538873531	5.88739398397200
Ga	5.82925966893309	8.10668236160433	6.01693870382673
Ga	13.46405462399724	13.68457398720471	6.03596220746721
H	12.70392634473740	8.66726173911075	5.87242512688768
H	1.92580493055856	13.03905179850334	2.77042456116366
H	9.62902520747314	18.48719934262444	2.80454881585007
H	9.62902510129696	13.04046301908156	2.76833071041630
H	9.62902482805826	7.59242111591102	2.73413529559633
H	0.77682473852687	11.44172602442631	3.92960753446929
H	14.62961383896615	11.44172606963624	3.92960796804970
Ga	7.71332081990106	16.35578722978040	3.87208080365776
Ga	7.73049684755730	10.91079569227291	3.84305783063562
Ga	7.70382243856032	5.30794427397511	3.94641455379809
Ga	7.70325650030277	21.84608093976547	3.88404337116975
Ga	3.82952589815123	16.36234936177156	3.86892033159722
Ga	3.82121796006162	10.87266811680734	3.86097523620222
H	4.62962024456213	5.99564052734048	3.89357733127922
Ga	11.58045972139984	16.35154657698631	3.87747505634486
Ga	11.58238134863331	10.86974951788346	3.86940250521509
H	10.77682058431842	5.99563915759321	3.89357711030490
Ga	1.94064626408682	13.68165963924862	6.01808694860505
H	2.70251348121952	8.66726136427560	5.87242544710939
H	8.84784140296041	3.22350896679282	5.83627576105587
Ga	9.60351238137502	19.12666285905485	5.98508737391736
Ga	9.63176339699002	13.63230155156498	6.01359752565091
Ga	9.60709764377919	8.11044536724057	5.99442661230293
H	0.74840063908602	11.67346250616433	7.64098896726481
H	14.65803976553757	11.67346261526636	7.64098959629012
Ga	7.70838560553682	16.67851789254257	7.54040258945260
Ga	7.88392792832765	10.91757604703630	7.66006939529084
Ga	7.71496365047630	5.12846213171959	8.51915810268702
Ga	7.70321940276993	22.19298211494136	7.44610025532413
Ga	3.91555431608558	16.74337858665111	7.49891113582965
Ga	3.62212656526200	11.11085530545364	7.54785116974308
H	4.60139082301270	6.22734722724684	7.60533346840915
Ga	11.49756051850209	16.72805670530319	7.49498047457920

Ga	11.67396008043321	11.17983411536239	7.55242029771906
H	10.80504974731532	6.22734635923083	7.60533301732932
P	5.78929424859290	17.71959786257991	4.00563432223050
P	5.76746181391447	12.27166114774578	3.96153988903098
P	5.79269973346013	6.82054617301961	3.94137761860250
H	6.38704559002170	22.71684348825861	4.00420320393921
H	12.85194064285652	17.25642362012172	3.96807756850682
P	13.48271404152961	12.28977628231539	3.98807417370007
P	5.81749753730432	17.88654202424742	8.10860406111646
P	5.77786096379298	12.11896304388059	7.76185915025734
P	5.79832316442424	6.91868231860302	7.98733369557996
H	6.39778589202994	22.90385776690871	7.89512877677785
H	12.85064302455422	17.45114201388239	7.85597215125042
P	13.55604916203830	12.44893241534565	8.09353472135484
H	7.70321978634589	4.53002827991134	2.61196080286770
H	7.70321993161557	20.84237166581509	2.68056180657161
H	7.70322006392034	15.40326646572720	2.65531095885539
H	7.70321994723545	9.95986306885203	2.62421696557316
H	3.85161014609230	15.39798381698810	2.64793601027809
H	3.85160998501964	9.96381137101968	2.62972782652303
H	11.55483002807531	15.39798435032865	2.64793740164938
H	11.55482985053873	9.96381204970821	2.62972873269828
H	2.55450137586594	17.25642190987809	3.96807773157390
P	1.92374031072210	12.28763829466126	3.98459282329515
P	9.62676857587656	17.72267034332603	4.00589477297505
P	9.65559037607125	12.29515425652834	3.98340609667476
P	9.61363035039358	6.81694316557989	3.93747317717537
H	9.01939450063643	22.71684277383909	4.00420264296504
H	0.63926657792497	14.47657186686841	5.89317729214871
H	14.76717399112370	14.47657314556046	5.89317633985514
P	7.70282066560840	4.09574661076850	6.01019514486425
P	7.70478569684912	20.48220787457724	5.90300445962672
P	7.72270994466673	15.01092863201789	5.90160264077874
P	7.71352129601482	9.54525290647536	5.77837124596100
H	4.48384906438519	19.92840924158733	5.92900074180445
P	3.87616970674136	15.01970864491305	5.90910046162147
P	3.84086593964308	9.50894452800824	5.85547430373077
H	10.92259276093100	19.92841066964207	5.92900142966302
P	11.52365827521396	15.01450506669171	5.90373693240925
P	11.57055952328037	9.52213291511103	5.87045686173021
H	2.55579641562776	17.45114121459498	7.85597177468505
P	1.83381048843140	12.46865335734638	8.10303832008479
P	9.59736447198081	17.88541993057535	8.10568569217854
P	9.68814837491310	12.34585452990454	8.06435565559436
P	9.60293520980129	6.91862404370587	7.96840669923531
H	9.00865301331531	22.90385829627741	7.89512909418695
O	7.73672383839952	9.44931847745855	9.18003568568641
H	8.49557660933668	8.81651779064632	9.14607411587076
H	6.93324599864059	8.88092879998158	9.11024499573871

H 5.72471699151000 12.96922441191478 8.88227992745135