The role of surface-bound dihydropyridine analogs in pyridine-catalyzed CO$_2$ reduction over semiconductor photoelectrodes

*Thomas P. Senfile,*$^a$ *Martina Lessio,*$^b$ and *Emily A. Carter*,$^c,*$

$a$ Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544-5263 (USA)  
$b$ Department of Chemistry, Princeton University, Princeton, NJ 08544-5263 (USA)  
$c$ School of Engineering and Applied Science, Princeton University, Princeton, NJ 08544-5263 (USA)

*eac@princeton.edu

Contents:

1) DFT Computational Details
2) Calculation of Standard Reduction Potentials
3) Cluster Models  
   • Figure S1: GaP, CdTe, and CuInS$_2$ cluster model geometries
4) Geometry of 2-PyH$^*$ on CdTe and CuInS$_2$  
   • Figure S2: Geometry of 2-PyH$^*$ adsorbed on reconstructed CdTe(111) and CuInS$_2$(112) surfaces  
   • Figure S3: Electron density difference of 2-PyH$^*$ adsorbed on CdTe(111) and CuInS$_2$(112) surfaces  
   • Figure S4: Transition state geometry for the reaction 2-PyH$^*$ + CO$_2$ $\rightarrow$ Py$^*$ + HCOO$^-$ on CdTe(111) and CuInS$_2$(112) surfaces
5) Impact of explicit solvation on SRP and HT barrier  
   • Figure S5: Geometry of 2-PyH$^*$ adsorbed on the reconstructed GaP(111), CdTe(111), and CuInS$_2$(112) surfaces with H$^+$, OH$^-$, or H$_2$O co-adsorbates  
   • Figure S6: Transition state geometry for the reaction 2-PyH$^*$ + CO$_2$ $\rightarrow$ Py$^*$ + HCOO$^-$ on GaP(111) with H$^+$, OH$^-$, and H$_2$O co-adsorbates
6) Reaction energy path for mechanism proceeding through DHP$^*$ intermediate  
   • Figure S7: Reaction energy diagrams for the reaction 2-PyH$^{**}$ + CO$_2$ $\rightarrow$ Py$^*$ + HCOO$^-$ proceeding though 2-PyH$^*$ and DHP$^*$ intermediates
7) Transition state for the HT reaction: H$^*$ + CO$_2$ $\rightarrow$ * + HCOO$^-$ on GaP(111)  
   • Figure S8: Transition state geometry for the reaction 2-PyH$^{**}$ + CO$_2$ $\rightarrow$ Py$^*$ + HCOO$^-$ on GaP(111)
8) Interaction between Py, H$_2$O and β-Ga$_2$O$_3$  
   • Figure S9: Adsorption of Py and H$_2$O on the β-Ga$_2$O$_3$(100) surface
7) Cartesian coordinates and total DFT energies of all reported geometries
1) DFT Computational Details

All computations were performed using the NWCHEM 6.6 simulation package\textsuperscript{1} with the hybrid B3LYP\textsuperscript{2,3} exchange-correlation (XC) functional and Grimme’s D2\textsuperscript{4} semi-empirical dispersion correction. Continuum solvation was treated with the “Solvation Model based on solute electron Density” (SMD),\textsuperscript{5} where the default NWCHEM parameters were employed for all atomic radii as well as for the dielectric constant of water ($\varepsilon = 78.4$). Inner core electrons/nuclei and outer-core/valence electrons of Ga, Cd, Te, Cu, and In were respectively represented by the following effective core potentials (ECPs) and double zeta (DZ) basis sets: Stuttgart (28, MWB) + DZ,\textsuperscript{6} Stuttgart (28, MWB) + DZ,\textsuperscript{7} Stuttgart (46, MWB) + DZ,\textsuperscript{6} Stuttgart (10, MWB) + DZ,\textsuperscript{8,9} and Stuttgart + DZ (46, MWB).\textsuperscript{6} The numbers in parentheses are the number of core electrons replaced by the ECP. MWB is the designation in the Stuttgart database indicating that the ECP is derived through fitting to multi-electron, quasi-relativistic data sets. Ga-(4s$^2$4p$^1$), Cd-(4s$^2$4p$^6$4d$^{10}$5s$^2$), Te-(5s$^2$5p$^4$), Cu-(3s$^2$3p$^6$3d$^{10}$4s$^1$), and In-(5s$^2$5p$^1$) outer-core/valence electrons were treated self-consistently. The Pople all-electron 6-31G** basis set\textsuperscript{10} was employed for all other atoms during geometry optimization and frequency analyses, and the Dunning all-electron aug-cc-pVDZ basis set\textsuperscript{11} was employed to refine single-point energies. Geometries were optimized with a quasi-Newton-Raphson algorithm (as available in NWCHEM 6.6) with a force convergence criterion of 0.00045 Ha bohr$^{-1}$. Minimum energy structures were verified with frequency analyses to ensure that all imaginary modes were eliminated. Transition state (TS) structures were also verified with frequency analyses, in which all reported TS structures have one imaginary frequency, and where optimization along both directions of the imaginary mode leads to minima corresponding to super-molecule structures characteristic of the reactant and product states (i.e., CO$_2$ and HCOO$^-$ weakly adsorbed above the 2-PyH$^+$ and Py$^+$.
surface models). Note that these super-molecule reactant states vary from the reference state used to determine the effective free energy barriers reported in the main text (i.e., there the effective reference state consists of CO$_{2(aq)}$ in solution at infinite separation from the surface). Numerical Hessians were employed to calculate frequencies, which were calculated with finite displacements ($\pm 0.01$ Å) of all atoms except the fixed pseudo-hydrogen saturators (see section 3 below).

2) Calculation of Standard Reduction Potentials (SRPs)

Standard reduction potentials were calculated from reaction free energies employing a previously established methodology.\textsuperscript{12,13} The SRP is calculated with the equation:

\[
E^0 = \frac{-\Delta G_{aq}}{nF} - \frac{mRT\ln(10)}{n}pH,
\]

where $E^0$ is the SRP, $n$ is the number of electrons transferred in the reduction, $m$ is the number of protons involved in the reaction, $F$ is the Faraday constant, $T$ is the temperature ($T = 298$ K at standard state), $R$ is the gas constant, and $pH = 5.2$. $\Delta G_{aq}$ is the reaction free energy, which is calculated with the expression:

\[
\Delta G_{aq} = G_{\text{reduced}} - G_{\text{reactant}} - n \cdot G_{e^-} - m \cdot G_{H^+},
\]

where $G_{\text{reduced}}$ and $G_{\text{reactant}}$ are the free energies of the reduced product and the reactant (including implicit solvation, as well as all translational, rotational, and vibrational contributions), respectively, and $G_{e^-}$ is the free energy of an electron in solution, as determined empirically from the standard hydrogen electrode (SHE = -4.281 V).\textsuperscript{14} $G_{H^+}$ is the free energy of a proton in solution, determined empirically as -11.72 eV.\textsuperscript{15} All reduction potentials are reported relative to the standard calomel electrode (0 V-SHE = -0.244 V-SCE). Statistical mechanical expressions for the ideal gas, harmonic oscillator, and rigid rotor were employed to derive translational, vibrational, and rotational thermochemical properties. Translational and rotational
contributions were considered to be zero for species adsorbed on cluster model surfaces with no translational or rotational degrees of freedom. The appropriateness of the employed implicit solvation model for calculating SRP values of the species considered in this study was demonstrated previously by Keith and Carter. The computed SRP for the reduction of \( \text{PyH}^{+} \) to \( \text{PyH}^{\bullet} \) using this approach is corroborated in the works of multiple separate research groups employing both theory\(^{17-19}\) and experiment,\(^{20}\) demonstrating the feasibility of this method. Finally, Keith and Carter\(^{21}\) further demonstrated that SRP values for the Py-derived species considered in this study calculated with B3LYP/aug-cc-pVDZ and with high level (U)CCSD(T)-F12/aug-cc-pVTZ-F12 approached varied by less than 0.1 V. Thus, the B3LYP functional is an appropriate choice for the calculation of adsorption energies and SRP values presented in this manuscript.

3) Cluster Models

GaP(111) and CdTe(111) surfaces were represented with the cluster models derived in our previous study.\(^{22}\) These models were cleaved from the periodic structures of a (2×2) reconstruction featuring one surface Ga/Cd vacancy per unit cell, as this reconstruction was predicted to be stable under photoelectrochemical conditions (Figure S1). The resulting clusters have 24 P/Te atoms, with 12 residing in the surface layer and 12 residing in the sub-surface layer. They have 21 Ga/Cd atoms, with nine residing in the surface layer and 12 in the sub-surface layer (i.e., the surface layer has one Ga/Cd vacancy per four P/Te atoms). Innocent dangling bonds at the cluster boundary were saturated using a pseudo-hydrogen capping scheme, in which each pseudo-hydrogen cap has a core charge modified to represent the atom-type it is replacing. Core charges of \( Z = +3/4 \text{ e} \), \( Z = +5/4 \text{ e} \), \( Z = +2/4 \text{ e} \), and \( Z = +6/4 \text{ e} \) are used when replacing Ga, P, Cd, and Te, respectively. The core charge is determined from the number of
valence electrons divided by the number of bonds in the stoichiometric bulk (i.e., for Ga there are three valence electrons divided by four bonds in the zinc blende structure). This stoichiometry yields a neutral singlet with no dangling bonds. The cluster model of the CuInS$_2$(112) surface was derived from the periodic geometry of a (2×2) surface reconstruction, in which there is one Cu$_{\text{In}}$ anti-site defect per (2×2) surface cell. This defect was predicted to be thermodynamically stable using the same methodology that was applied to the GaP and CdTe surfaces.$^{23}$ The resulting cluster has 12 Cu atoms, four In atoms, and 16 S atoms in the surface layer, and has eight Cu atoms, eight In atoms, and 16 S atoms in the sub-surface layer (i.e., there are four Cu$_{\text{In}}$ anti-site defects in the equivalent (4×4) surface layer). Pseudo-hydrogen saturators were employed with core charges of $Z = +1/4 \, e$, $Z = +3/4 \, e$, and $Z = +6/4 \, e$ when replacing Cu, In, and S, respectively. Pseudo-hydrogens were positioned by replacing a cation/anion in the geometry of the optimized extended surface, followed by an optimization of all pseudo-hydrogen bond lengths (where all atoms in the cluster are frozen and pseudo-hydrogen saturators are relaxed along their bond to the nearest atom in the cluster). Pseudo-hydrogens were then frozen in these positions during all subsequent geometry optimizations and vibrational frequency calculations. We note that these models of the surface assume that restructuring of the surface caused by exposure to visible light and the applied voltage is negligible. The voltages applied in the photo-electrochemical experiments are generally low—with the onset of Py-enhanced CO$_2$ reduction demonstrated to occur at potentials as low as -0.2 V vs. SCE.$^{24}$ We therefore do not expect that voltage-induced restructuring of the surface will play a significant role in these systems.

The cluster model approach was extensively benchmarked and validated by Keith et al.$^{13}$ where it was demonstrated that the cluster model approach yields adsorption energies that are
very similar to those computed with a periodic surface model. The cluster model approach was further refined, extended, and validated by Senftle et al.\textsuperscript{22,23} These studies show that the cluster models yield adsorption energies that are typically within \(-0.2\) eV of the values computed with periodic surface models. These studies also show that the B3LYP XC functional yields adsorption energies consistent with the widely used PBE\textsuperscript{25} XC functional.

\textbf{Figure S1.} Top (left) and (right) side views of the cluster models representing the reconstructed (a) GaP(111)-Ga\textsubscript{vac}, (b) CdTe(111)-Cd\textsubscript{vac}, and (c) CuInS\textsubscript{2}(112)-Cu\textsubscript{In} surfaces. Subsurface atoms
are omitted in top views for clarity. Core charge of pseudo-hydrogen saturators are indicated with color-coded labels.

4) Geometry of 2-PyH* on CdTe and CuInS₂

Figure S2. Side view of the geometry of 2-PyH* adsorbed on the reconstructed (a) CdTe(111) and (b) CuInS₂(112) surfaces. Pseudo-hydrogen saturators are omitted for clarity.
Figure S3. Electron density difference of 2-PyH⁺ adsorbed on the reconstructed (a) CdTe(111) and (b) CuInS₂(112) surfaces. The red (blue) isosurface indicates electron density depletion (accumulation), and the isosurface level corresponds to 0.003 e⁻ bohr⁻¹.
**Figure S4.** Side view of the TS geometry of a HT from the 2-PyH⁺ intermediate to CO₂ over the (a) CdTe(111) and (b) CuInS₂(112) surfaces. Pseudo-hydrogen saturators are omitted for clarity.

---

5) Impact of explicit solvation on SRP and HT barrier

**Figure S5.** (a-b) Top (left) and side (right) view of the geometry of 2-PyH⁺ adsorbed on the reconstructed GaP(111) surface with (a) a co-adsorbed H⁺ and (b) a co-adsorbed 2H₂O, 2OH⁻, and 2H⁺ layer. (c) Top (left) and side (right) view of the geometry of 2-PyH⁺ adsorbed on the reconstructed CdTe(111) surface with a co-adsorbed 4H₂O layer. (d) Top (left) and side (right)
view of the geometry of 2-PyH$^{*}$ adsorbed on the reconstructed CuInS$_2$(112) surface with co-adsorbed 6H$_2$O layer. Pseudo-hydrogen saturators are omitted for clarity.

**Figure S6.** Top view of the TS geometry of a HT from the 2-PyH$^{*}$ intermediate to CO$_2$ over the reconstructed GaP(111) surface in the presence of an explicit solvation layer (in addition to implicit solvation). The structure of the solvation layer was determined in a previous study.$^{22}$ Pseudo-hydrogen saturators are omitted for clarity.

For further information regarding the impact of explicit solvation, included in addition to implicit solvation, we refer the reader to previous work reported by Lessio et al.$^{26,27}$ For information regarding the interaction between water and the reconstructed GaP, CdTe, and CuInS$_2$ surface, we refer the reader to work reported by Senftle et al.$^{22,23}$ Finally, for further experimental and theoretical work investigating the nature of Py, H$_2$O, H$^+$, and OH$^-$ adsorption on GaP, we refer the reader to Kronawitter et al.$^{28,29}$

6) Reaction energy diagrams for mechanisms proceeding through 2-PyH$^{*}$ or DHP$^*$
**Figure S7.** CO$_2$ reduction pathways proceeding through HT from surface-bound 2-PyH$^*$ (blue) or DHP* (orange) intermediates on GaP(111). Species labeled with an * are adsorbed on the surface. (Inset) Side view of the TS-(DHP* + CO$_2$) transition state structure.

In the above diagram we present the reaction free energy paths for two possible mechanisms for the overall reaction over the reconstructed GaP(111) surface:

$$2\text{-PyH}^* + \text{H}^+_{(aq)} + \text{CO}_2(aq) \rightarrow \text{Py}^* + \text{HCOOH}_{(aq)}$$

The first mechanism proceeds via an initial protonation of 2-PyH$^*$ forming DHP*, followed by a HT from DHP* to CO$_2(aq)$ yielding HCOO$^-$$_{aq}$ and PyH$^+$*, then completed by a proton transfer from PyH$^+$* to HCOO$^-$$_{aq}$ to obtain Py$^*$ and HCOOH$_{(aq)}$:

1. **$2\text{-PyH}^* + \text{H}^+_{(aq)} \rightleftharpoons \text{DHP}^*$** \hspace{1cm} $\Delta G^1 = -0.60 \text{ eV (pH = 5.2)}$
2. **$\text{DHP}^* + \text{CO}_2(aq) \rightarrow \text{HCOO}^-_{aq} + \text{PyH}^+*$** \hspace{1cm} $\Delta G^2 = -0.28 \text{ eV, } \Delta G^{TS} = 1.25 \text{ eV}$
3. **$\text{PyH}^+* + \text{HCOO}^-_{aq} \rightleftharpoons \text{HCOOH}_{(aq)} + \text{Py}^*$** \hspace{1cm} $\Delta G^3 = -0.31 \text{ eV}$

$\Delta G^1$, $\Delta G^2$, and $\Delta G^3$ correspond to the reaction free energies of steps (1), (2), and (3), respectively, and $\Delta G^{TS}$ corresponds to the free energy barrier for the rate-limiting HT step. The apparent barrier for this mechanism is 0.65 eV, as shown in orange in Figure S7. This barrier is computed relative to a reference state that corresponds with $2\text{-PyH}^* + \text{H}^+_{(aq)} + \text{CO}_2(aq)$, and therefore assumes that step (1) is in equilibrium. This can be considered as the “best case” scenario yielding the lowest possible apparent barrier for this reaction path. Because $\Delta G^1$ is very exergonic and the reaction is carried out at room temperature, the apparent barrier instead will likely resemble the $\Delta G^{TS}$ of step (2), which would be indicative of the system becoming trapped.
in the intermediate DHP* state. The above path can be directly compared to the barrier for the second reaction path featuring a direct HT from 2-PyH*, as proposed in Scheme 1 of the main text:

\[
\begin{align*}
(1) \quad 2\text{-PyH}^* + \text{CO}_2^{(aq)} & \rightarrow \text{Py}^* + \text{HCOO}^{(aq)} \quad \Delta G^1 = -1.42 \text{ eV}, \Delta G^{TS} = 0.59 \text{ eV} \\
(2) \quad \text{H}^+^{(aq)} + \text{HCOO}^{(aq)} & \rightleftharpoons \text{HCOOH}^{(aq)} \quad \Delta G^2 = 0.23 \text{ eV (pH = 5.2)}
\end{align*}
\]

This mechanism yields an apparent barrier of 0.59 eV—commensurate with the “best case” barrier for reaction path proceeding through the DHP* intermediate, where the latter would only be observed at elevated temperatures not practical in this system.

**7) Transition state for the reaction: H^* + CO_2 \rightarrow * + HCOO^- on GaP(111)**

*Figure S8.* Side view of the TS geometry of a HT directly from the reconstructed GaP(111) surface. Pseudo-hydrogen saturators are omitted for clarity.

**8) Interaction between Py, H_2O and β-Ga_2O_3**

In this section we consider the possible role of a native surface oxide on the photo-electrode surface. The GaP surfaces employed in the photo-electrochemical CO_2 reduction
experiments were pre-treated with aggressive etchants that would remove any native oxide on the surface. Furthermore, the electrodes are operated under cathodic conditions that would not favor the re-formation a native oxide layer. Ziegler et al.\textsuperscript{30} provide experimental evidence demonstrating the removal of a native oxide from p-type GaP via an etching procedure similar to the procedure employed by Bocarsly and co-workers in the original CO$_2$ reduction experiments.\textsuperscript{24} Nevertheless, surface regions with a thin oxide layer may persist, and as such we have investigated possible ways in which a native oxide could impact that surface-bound reaction mechanism presented in this work. Here we only consider Ga$_2$O$_3$ oxide structures because the oxidation of surface P atoms will not impact Py binding at Ga metal sites, and because native Ga$_2$O$_3$ was observed by Ziegler et al.\textsuperscript{30} to form on p-GaP electrode surfaces. We employ a slab model of the low-index (100) surface orientation of β-Ga$_2$O$_3$, as this is the most stable surface of β-Ga$_2$O$_3$ (see Bermudez\textsuperscript{31} for a comparison of different Ga$_2$O$_3$ surface structures and energies), which in turn is the most stable polymorph of Ga$_2$O$_3$. To test the strength of such dative bonds on the native oxide, we calculated the adsorption energy of Py and H$_2$O at the undercoordinated Ga site on Ga$_2$O$_3$(100), where we employ a (2×2) periodic surface model, the PBE XC functional,\textsuperscript{25} and a 4×4×1 Monkhorst-Pack\textsuperscript{32} k-point mesh with all other computational settings identical to those described in our previous work.\textsuperscript{22} The calculated adsorption energies of Py and H$_2$O are $\Delta E_{\text{ads}} = -0.96$ eV and $\Delta E_{\text{ads}} = -0.67$ eV, respectively.
Figure S9. (a) Side view of $\beta$-Ga$_2$O$_3$(100) surface, on which there is an open coordination site at the octahedral $d^{10}$ metal center of the surface Ga atom. (b-c) Optimized adsorption geometry of (b) Py and (c) H$_2$O on the $\beta$-Ga$_2$O$_3$(100) surface forming donor-acceptor bonds at the open coordination site. Cartesian coordinates are provided in Section 9. Adsorption energies calculated with the formulae: $\Delta E_{\text{ads}} = E[\text{Py/Ga}_2\text{O}_3(100)] - E[\text{Py}] - E[\text{Ga}_2\text{O}_3(100)]$ or $\Delta E_{\text{ads}} = E[\text{H}_2\text{O/Ga}_2\text{O}_3(100)] - E[\text{H}_2\text{O}] - E[\text{Ga}_2\text{O}_3(100)]$.

References
(1) Valiev, M.; Bylaska, E. J.; Govind, N.; Kowalski, K.; Straatsma, T. P.; Van Dam, H. J. J.; Wang, D.; Nieplocha, J.; Apra, E.; Windus, T. L.; de Jong, W. A. NWCHEM: A Comprehensive and Scalable Open-Source Solution for Large Scale Molecular Simulations. *Comput. Phys. Commun.* 2010, 181, 1477-1489.
(2) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phys. Rev. B* 1988, 37, 785-789.
(3) Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A* 1988, 38, 3098-3100.
(4) Grimme, S. Semiempirical GGA-Type Density Functional Constructed with a Long-Range Dispersion Correction. *J. Comput. Chem.* 2006, 27, 1787-1799.
(5) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* 2009, 113, 6378-6396.
(6) Bergner, A.; Dolg, M.; Küchle, W.; Stoll, H.; Preuß, H. Ab Initio Energy-Adjusted Pseudopotentials for Elements of Groups 13–17. *Mol. Phys.* **1993**, *80*, 1431-1441.

(7) Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H. Energy-Adjusted Ab Initio Pseudopotentials for the Second and Third Row Transition Elements. *Theoretica chimica acta* **1990**, *77*, 123-141.

(8) Dolg, M.; Wedig, U.; Stoll, H.; Preuss, H. Energy-Adjusted Ab Initio Pseudopotentials for the First Row Transition Elements. *J. Chem. Phys.* **1987**, *86*, 866-872.

(9) Martin, J. M. L.; Sundermann, A. Correlation Consistent Valence Basis Sets for Use with the Stuttgart–Dresden–Bonn Relativistic Effective Core Potentials: The Atoms Ga–Kr and in–Xe. *J. Chem. Phys.* **2001**, *114*, 3408-3420.

(10) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. Self-Consistent Molecular Orbital Methods. Xxiii. A Polarization-Type Basis Set for Second-Row Elements. *J. Chem. Phys.* **1982**, *77*, 3654-3665.

(11) Dunning, T. H. Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron through Neon and Hydrogen. *J. Chem. Phys.* **1989**, *90*, 1007-1023.

(12) Keith, J. A.; Carter, E. A. Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO$_2$. *J. Am. Chem. Soc.* **2012**, *134*, 7580-7583.

(13) Keith, J.; Muñoz-García, A.; Lessio, M.; Carter, E. Cluster Models for Studying CO$_2$ Reduction on Semiconductor Photoelectrodes. *Top. Catal.* **2015**, *58*, 46-56.

(14) Isse, A. A.; Gennaro, A. Absolute Potential of the Standard Hydrogen Electrode and the Problem of Interconversion of Potentials in Different Solvents. *J. Phys. Chem. B* **2010**, *114*, 7894-7899.

(15) Tossell, J. A. Calculation of the Properties of Molecules in the Pyridine Catalyst System for the Photochemical Conversion of CO$_2$ to Methanol. *Comput. and Theor. Chem.* **2011**, *977*, 123-127.

(16) Senftle, T. P.; Lessio, M.; Carter, E. A. Interaction of Pyridine and Water with the Reconstructed Surfaces of GaP(111) and CdTe(111) Photoelectrodes: Implications for CO$_2$ Reduction. *Chem. Mater.* **2016**, *28*, 5799-5810.

(17) Senftle, T. P.; Carter, E. A. Theoretical Determination of Band Edge Alignments at the Water–CulnS$_2$(112) Semiconductor Interface. *Langmuir* **2017**, doi: 10.1021/acs.langmuir.7b00668.

(18) Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.
(26) Lessio, M.; Senftle, T. P.; Carter, E. A. Is the Surface Playing a Role During Pyridine-Catalyzed CO₂ Reduction on p-Gap Photoelectrodes? *ACS Energy Lett.* 2016, 1, 464-468.

(27) Lessio, M.; Riplinger, C.; Carter, E. A. Stability of Surface Protons in Pyridine-Catalyzed CO₂ Reduction at p-GaP Photoelectrodes. *Phys. Chem. Chem. Phys.* 2016, 18, 26434-26443.

(28) Kronawitter, C. X.; Lessio, M.; Zhao, P.; Riplinger, C.; Boscoboinik, A.; Starr, D. E.; Sutter, P.; Carter, E. A.; Koel, B. E. Observation of Surface-Bound Negatively Charged Hydride and Hydroxide on GaP(110) in H₂O Environments. *J. Phys. Chem. C* 2015, 119, 17762-17772.

(29) Kronawitter, C. X.; Lessio, M.; Zahl, P.; Muñoz-García, A. B.; Sutter, P.; Carter, E. A.; Koel, B. E. Orbital-Resolved Imaging of the Adsorbed State of Pyridine on GaP(110) Identifies Sites Susceptible to Nucleophilic Attack. *J. Phys. Chem. C* 2015, 119, 28917-28924.

(30) Ziegler, J.; Fertig, D.; Kaiser, B.; Jaegermann, W.; Blug, M.; Hoch, S.; Busse, J. Preparation and Characterization of GaP Semiconductor Electrodes for Photoelectrochemical Water Splitting. *Energy Procedia* 2012, 22, 108-113.

(31) Bermudez, V. M. The Structure of Low-Index Surfaces of β-Ga₂O₃. *Chem. Phys.* 2006, 323, 193-203.

(32) Monkhorst, H. J.; Pack, J. D. Special Points for Brillouin-Zone Integrations. *Phys. Rev. B* 1976, 13, 5188-5192.

9) Cartesian coordinates and total DFT energies of all reported geometries

All geometries are provided in cartesian coordinates (Å). Core charges (units of e) of pseudo-hydrogen saturators are indicated in brackets.

**GaP(111) Cluster Model:**

**Total DFT Energy:** -8254.24050487618 Ha

| H[Z=1.25] | -7.16917963 | -1.86191902 | -1.50875678 |
| H[Z=1.25] | -7.12359105 | -4.05277974 | 1.45967287 |
| H[Z=1.25] | -5.21877988 | -5.27186105 | -1.50210210 |
| H[Z=1.25] | -1.93616368 | 7.12039741 | -1.52727102 |
| H[Z=1.25] | 5.17649945 | -5.31343078 | -1.50257282 |
| H[Z=1.25] | 0.03308891 | 8.34359116 | 1.42738567 |
| H[Z=1.25] | 1.99229336 | 7.10424815 | -1.52701504 |
| H[Z=1.25] | 7.15424499 | -1.91909686 | -1.50983857 |
| H[Z=1.25] | 7.09104932 | -4.10925328 | 1.45902848 |
| H[Z=0.75] | -7.04080034 | 1.80643186 | -1.29546678 |
| H[Z=0.75] | -5.86917827 | 1.12364620 | -3.24865470 |
| H[Z=0.75] | -1.98298596 | -5.66960819 | -3.23539736 |
| H[Z=0.75] | -1.99138426 | -7.01801045 | -1.27867655 |
| H[Z=0.75] | -3.89552936 | 4.51095106 | -3.25417630 |
| H[Z=0.75] | -5.06431158 | 5.19968792 | -1.30186433 |
| H[Z=0.75] | -5.11881160 | 3.03326049 | 1.48221186 |
| H[Z=0.75] | -0.00933709 | -2.28230504 | -3.24178295 |
| H[Z=0.75] | 1.95706118 | 1.09255459 | -3.24857649 |
| H[Z=0.75] | -1.94885853 | 1.10807425 | -3.24796642 |
| H[Z=0.75] | -0.02380254 | -5.97733262 | 1.50670662 |
| H[Z=0.75] | 1.93518640 | -7.03632094 | -1.27798518 |
| H[Z=0.75] | 1.93733378 | -5.68518013 | -3.23470908 |
| H[Z=0.75] | 3.93070915 | 4.47985638 | -3.25539508 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| H       | 5.10416108 | 5.15874627 | -1.30275722|
| H       | 7.05519723 | 1.75097329 | -1.29567388|
| H       | 5.14326766 | 2.99303266 | 1.48174557 |
| H       | 5.87738005 | 1.07698214 | -3.24789021|
| H       | -3.92262892| -2.27080813| -3.23296450|
| H       | 3.90391917 | -2.30244238| -3.2324523  |
| H       | 0.01757191 | 4.49108197 | -3.24614510|
| Ga      | -5.84661933| -1.09920206| -0.98456779|
| Ga      | -3.90029554| -4.51165063| -0.97995274|
| Ga      | -5.70579606| -3.26433655| 1.61018402 |
| Ga      | -3.86233258| 2.23482566 | -1.05243133|
| Ga      | -1.94210938| 5.60941681 | -1.00133280|
| Ga      | 0.00921050 | 2.23894040 | 0.96092221 |
| Ga      | -3.96052871| -0.11602717| 1.63849844 |
| Ga      | -1.95461305| -1.13916078| -0.96385777|
| Ga      | -1.84054278| 3.55870123 | 1.61613881 |
| Ga      | -0.01736303| -4.50042985| -1.02870032|
| Ga      | 1.94632262 | -1.15425761| -0.96452758|
| Ga      | -2.12406000| -3.37228023| 1.63089164 |
| Ga      | 3.86352163 | -4.54254352| -0.97875063|
| Ga      | 2.09662172 | -3.38313194| 1.63037014 |
| Ga      | 0.02694395 | 6.69269566 | 1.55332311 |
| Ga      | 1.98666137 | 5.59358046 | -1.00092376|
| Ga      | 3.87953034 | 2.20476164 | -1.05274053|
| Ga      | 1.86784508 | 3.54428552 | 1.61641016 |
| Ga      | 3.96182192 | -0.14488879| 1.63892950 |
| Ga      | 5.83861889 | -1.1448636 | -0.98580291|
| Ga      | 5.67993614 | -3.30890895| 1.61140101 |
| P       | -6.12722130| -0.98202296| 1.45669857 |
| P       | -5.85550677| 1.13328809 | -1.79975827|
| P       | -3.96414313| -4.80280259| 1.46281993 |
| P       | -3.92037508| -2.26399361| -1.77861209|
| P       | -1.97461257| -5.65543390| -1.78527005|
| P       | -3.89151014| 4.50491963 | -1.80441139|
| P       | -2.16017112| 5.87062471 | 1.43089598 |
| P       | -3.87169495| 2.28394570 | 1.36646627 |
| P       | -0.00877504| -2.26512887| -1.78931130|
| P       | 0.00836946 | 2.16806067 | 1.48924070 |
| P       | -1.92975658| 1.10468786 | -1.79657554|
| P       | 1.83327719 | -1.08132535| 1.48603603 |
| P       | 0.01766220 | 4.49667072 | -1.79344264|
| P       | -0.01755305| -4.51996900| 1.38824613 |
| P       | 1.93838799 | 1.08924441 | -1.79735822|
| P       | -1.84186049| -1.07469892| 1.48617344 |
| P       | 3.92387024 | -4.83149977 | 1.46403734 |
| P       | 1.92981600 | -5.67300905| -1.78441656 |
|   |        |        |        |
|---|---|---|---|
| P | 3.90281381 | -2.29501495 | -1.77821880 |
| P | 3.92587579 | 4.47406553 | -1.80572859 |
| P | 3.88983887 | 2.25485926 | 1.36599791 |
| P | 2.20714591 | 5.85339105 | 1.43080576 |
| P | 5.86409497 | 1.08808832 | -1.79936483 |
| P | 6.12083043 | -1.03015006 | 1.45511557 |

_CdTe(111) Cluster Model:_

_Total DFT Energy: -3736.045677928867 Ha_

|   |        |        |        |
|---|---|---|---|
| H[Z=1.50] | -1.75138259 | -8.59767089 | -1.62855290 |
| H[Z=1.50] | 0.67037618 | -9.68021338 | 1.89792430 |
| H[Z=1.50] | 2.92144564 | -8.27366002 | -1.62876616 |
| H[Z=1.50] | 8.32190144 | 2.78296660 | -1.62896305 |
| H[Z=1.50] | -8.71723167 | 4.25750973 | 1.89718348 |
| H[Z=1.50] | -6.59451414 | 5.81604226 | -1.62901244 |
| H[Z=1.50] | 5.70417563 | 6.66756438 | -1.62859999 |
| H[Z=1.50] | 8.04652933 | 5.42077113 | 1.89711165 |
| H[Z=1.50] | -8.63051339 | 1.60104928 | -1.62466316 |
| H[Z=0.50] | -5.65534902 | -6.63734007 | -1.37291300 |
| H[Z=0.50] | -4.28657630 | -5.70417316 | -3.77447264 |
| H[Z=0.50] | 5.03384280 | -5.05797325 | -3.77589806 |
| H[Z=0.50] | 0.37363043 | -5.38107397 | -3.74268535 |
| H[Z=0.50] | 6.51795185 | -5.79268882 | -1.37301110 |
| H[Z=0.50] | -6.89770712 | -1.82899976 | -3.77385721 |
| H[Z=0.50] | -8.27585199 | -2.74678081 | -1.37280002 |
| H[Z=0.50] | 2.42291977 | -1.18266106 | -3.77428562 |
| H[Z=0.50] | -0.18619891 | 2.69084977 | -3.77442204 |
| H[Z=0.50] | -4.84641206 | 2.36774853 | -3.74170832 |
| H[Z=0.50] | -2.23631846 | -1.50631492 | -3.77507182 |
| H[Z=0.50] | 8.57630985 | -1.57859950 | -1.37311172 |
| H[Z=0.50] | 4.47400676 | 3.01394833 | -3.74063576 |
| H[Z=0.50] | 7.08430921 | -0.85997569 | -3.77500021 |
| H[Z=0.50] | -0.49626403 | 7.14712653 | 1.92122225 |
| H[Z=0.50] | -2.79698383 | 6.56595354 | -3.77380959 |
| H[Z=0.50] | -2.92074490 | 8.22064343 | -1.37250560 |
| H[Z=0.50] | 6.43813024 | -3.14515854 | 1.92158494 |
| H[Z=0.50] | 1.75908733 | 8.54181707 | -1.37396620 |
| H[Z=0.50] | 1.86426608 | 6.88884632 | -3.77577120 |
| H[Z=0.50] | -5.94435086 | -4.00383630 | 1.92191098 |
| Cd | -1.89458200 | -6.79919740 | -1.02087214 |
| Cd | 2.81889624 | -6.46928454 | -1.01367521 |
| Cd | -1.85096320 | -4.27389105 | 1.74759816 |
| Cd | 0.54155304 | -7.72941846 | 1.82403834 |
| Cd | 2.41899701 | -3.98750839 | 1.72764337 |
| Cd | -4.43179588 | -2.98300771 | -1.02876286 |
| Cd | -7.01001264 | 0.79665685 | -1.01117974 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Cd      | -2.38003717 | 1.16960290 | -1.02030700|
| Cd      | -6.95615116 | 3.40012497 | 1.80208215 |
| Cd      | 0.17853711  | -2.64124723 | -1.01628324|
| Cd      | -4.66776536 | -0.11574601 | 1.73384775 |
| Cd      | 4.80627674  | -2.34093156 | -1.03013350|
| Cd      | 2.19279520  | 1.47598430  | -1.01933909|
| Cd      | -2.80130198 | 3.75715612  | 1.72794048 |
| Cd      | 6.82778616  | 1.76835158  | -1.00767598|
| Cd      | 2.24666636  | 4.10583040  | 1.73605893 |
| Cd      | 4.66415577  | 0.52946166  | 1.73689478 |
| Cd      | 6.41347131  | 4.33139061  | 1.81501472 |
| Cd      | -4.93815681 | 5.04301656  | -1.00805026|
| Cd      | -0.36827297 | 5.33396609  | -1.03174338|
| Cd      | 4.19199365  | 5.67335683  | -1.01044827|
| Te      | -2.11287996 | -7.03821702 | 1.82556782 |
| Te      | -4.29573971 | -5.67856539 | -2.00213737|
| Te      | 3.07568764  | -6.68470526 | 1.82694035 |
| Te      | 0.37389100  | -5.36365348 | -1.93864723|
| Te      | 5.04051300  | -5.02968404 | -2.00331180|
| Te      | -6.87761282 | -1.84631982 | -2.00198762|
| Te      | -7.32716305 | 0.68482439  | 1.82755614 |
| Te      | -4.44209215 | -2.99312222 | 1.82090080 |
| Te      | 2.41267832  | -1.18141356 | -2.00491719|
| Te      | -2.18217091 | 1.07352997  | 1.82757630 |
| Te      | -2.22958483 | -1.49544227 | -2.00517439|
| Te      | 2.03301487  | 1.35911631  | 1.83003271 |
| Te      | -4.83870041 | 2.36750239  | -1.93679987|
| Te      | 4.81137678  | -2.35265099 | 1.81789571 |
| Te      | -0.18522496 | 2.68305476  | -2.00607077|
| Te      | 0.16910790  | -2.40251486 | 1.83048977 |
| Te      | 7.18051665  | 1.70019763  | 1.82911878 |
| Te      | 7.06961063  | -0.87030550 | -2.00092862|
| Te      | 4.45744680  | 3.01004857  | -1.93733995|
| Te      | -2.77241071 | 6.56364565  | -2.00153277|
| Te      | -0.37296079 | 5.34039617  | 1.81602962 |
| Te      | -5.05398349 | 5.37547459  | 1.82840623 |
| Te      | 1.84020478  | 6.88210633  | -2.00453130|
| Te      | 4.25705907  | 6.02097009  | 1.82754531 |

CulnS$_2$(112) Cluster Model:

Total DFT Energy: -16746.220389022201 Ha
| Z            | x          | y          | z          |
|--------------|------------|------------|------------|
| H[Z=0.25]    | 2.63494940 | 7.19964107 | -3.37069240 |
| H[Z=0.25]    | -0.13025308| 0.99322361 | -3.54484812 |
| H[Z=0.25]    | 3.49089212 | -0.71040898| -3.30452282 |
| H[Z=0.25]    | 0.72573547 | -6.91682583| -3.47931789 |
| H[Z=0.25]    | 1.95505660 | -8.08608437| 1.61050420  |
| H[Z=0.25]    | 7.58790846 | 5.75381088 | -0.67633629 |
| H[Z=0.25]    | 6.03585088 | 7.78705249 | 1.92396976  |
| H[Z=0.25]    | 6.63554540 | 1.72940552 | -3.05973321 |
| H[Z=0.25]    | 8.44227276 | -2.15641529| -0.61092269 |
| H[Z=0.25]    | 6.89179349 | -0.12299656| 1.99013933  |
| H[Z=0.25]    | 7.49148801 | -6.18064354| -2.99356364 |
| H[Z=0.75]    | -5.01843397| 7.43705641 | -1.89309912 |
| H[Z=0.75]    | -3.70200274| 2.61262913 | -3.43312293 |
| H[Z=0.75]    | -2.84606023| -5.29741893| -3.36695337 |
| H[Z=0.75]    | -0.51951939| 4.85791074 | -3.20575230 |
| H[Z=0.75]    | 1.74731758 | 8.17323860 | -1.40734493 |
| H[Z=0.75]    | 3.06374980 | 3.34881142 | -2.94736868 |
| H[Z=0.75]    | 0.33642333 | -3.05213931| -1.3958272 |
| H[Z=0.75]    | 3.91969231 | -4.56123664| -2.88119911 |
| H[Z=0.75]    | 0.06568361 | -8.04935328| -1.43633678 |
| H[Z=0.75]    | 6.08154564 | 3.83922735 | 1.83089602  |
| H[Z=0.75]    | 6.24623315 | 5.59409303 | -2.71999805 |
| H[Z=0.75]    | 6.93748836 | -4.07082270| 1.89706560  |
| H[Z=0.75]    | 7.10217587 | -2.31595702| -2.6538247 |
| H[Z=0.75]    | 7.72546971 | 1.84435129 | -0.96856027 |
| H[Z=0.75]    | 6.83143615 | -7.31317099| -0.95058252 |
| H[Z=0.75]    | 8.58141233 | -6.06569776| -0.90239070 |
| Cu           | -3.15543611| 4.75214249 | 1.25962450  |
| Cu           | -5.21645780 | 4.43302878 | -1.32328542 |
| Cu           | -2.66229125 | 0.76031221 | 1.26024883  |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Cu      | -6.87263050 | 6.44235022 | 0.92229489 |
| Cu      | -2.28479210 | -3.24257099 | 1.26122717 |
| Cu      | -4.37230164 | -3.43259532 | -1.27323240 |
| Cu      | -1.74073404 | -7.17405459 | 1.26653739 |
| Cu      | -6.03259825 | -1.59501052 | 0.96041321 |
| Cu      | 3.61050433  | 5.55993283  | 1.76903901 |
| Cu      | 1.53295000  | 5.19303777  | -0.81674610 |
| Cu      | 4.08048580  | 1.47756834  | 1.71607071 |
| Cu      | -1.59593235 | 2.78009129  | -1.03391158 |
| Cu      | -0.5501253  | 7.15346126  | 1.3893270 |
| Cu      | 4.46505295  | -2.37814355 | 1.74031674 |
| Cu      | 2.35728641  | -2.63308629 | -0.77340859 |
| Cu      | 4.99876975  | -6.44441151 | 1.73454566 |
| Cu      | -0.71490460 | -5.05625596 | -0.97806947 |
| Cu      | 0.72546718  | -0.84290556 | 1.53219635 |
| Cu      | 4.99198459  | 3.54494782  | -0.58757191 |
| Cu      | 5.88110453  | -4.29467291 | -0.53346414 |
| In      | -6.39548505 | 2.47176132  | 0.86408039 |
| In      | -5.53875132 | -5.43803134 | 0.95089555 |
| In      | -4.67814147 | 0.48076693  | -1.57214989 |
| In      | -3.85004433 | -7.39302419 | -1.50478950 |
| In      | -2.11606083 | 6.67840359  | -1.22944853 |
| In      | 0.40781662  | 3.19222951  | 1.60667926 |
| In      | -1.24128491 | -1.11041813 | -1.20477589 |
| In      | 1.32343272  | -4.72714352 | 1.67792368 |
| In      | 1.96651521  | 1.15272206  | -1.07521850 |
| In      | 2.79862970  | -6.67010843 | -1.03650671 |
| In      | 4.65410652  | 7.41293118  | -0.70221956 |
| In      | 5.56081073  | -0.34105597 | -0.71758693 |
| S       | -5.45457757 | 4.62766860  | 1.09118264 |
| S       | -4.98198999 | 0.47818983  | 0.92019861 |
| S       | -3.74857575 | 2.66860571  | -2.03545343 |
| S       | -4.27994870 | 6.34777779  | -2.33748175 |
| S       | -4.56176390 | -3.30388303 | 1.15677877 |
| S       | -4.05996092 | -7.42035126 | 0.94751035 |
| S       | -2.89284443 | -5.22628112 | -1.97331540 |
| S       | -3.45902978 | -1.49643632 | -2.2539864 |
| S       | -0.30309358 | 1.00906005  | -1.99307551 |
| S       | 1.34600962  | 5.36595141  | 1.54748130 |
| S       | -0.62586263 | 4.83406436  | -1.81517872 |
| S       | 1.78705721  | 1.19761708  | 1.40099386 |
| S       | 2.88400017  | 3.36571024  | -1.57485210 |
| S       | 2.50737758  | 7.09811502  | -1.85187690 |
| S       | -2.30281126 | 6.87576340  | 1.16625331 |
| S       | -1.93916773 | 2.86580960  | 1.35386057 |
| S       | 0.54115235  | -6.84878865 | -1.94938269 |
| S   | 2.20979171  | -2.54239890  | 1.60264718  |
| S   | 0.22016395  | -3.02509133  | -1.74784548 |
| S   | 2.70665834  | -6.73139016  | 1.42253207  |
| S   | 3.76082602  | -4.49772818  | -1.51576671 |
| S   | 3.35542326  | -0.72571758  | -1.76447820 |
| S   | -1.48561844 | -1.13736014  | 1.23350311  |
| S   | -1.01859980 | -5.07992807  | 1.41034109  |
| S   | 6.44078914  | 1.81953112   | -1.51945334 |
| S   | 6.14675013  | 5.56771995   | -1.32832786 |
| S   | 4.51998759  | 7.66148852   | 1.67079636  |
| S   | 4.72909629  | 3.62266785   | 1.77275865  |
| S   | 7.28809739  | -6.08323175  | -1.42947975 |
| S   | 6.99854217  | -2.29649222  | -1.26374762 |
| S   | 5.40745779  | -0.33557903  | 1.70389351  |
| S   | 5.59299096  | -4.31052876  | 1.84034844  |

**Py* on GaP(111):**

Total DFT Energy: -8502.604923179146 Ha

| H[Z=1.25] | 1.95820894  | -7.37142164  | -1.18662511 |
| H[Z=1.25] | 4.15694083  | -7.08333694  | 1.76229146  |
| H[Z=1.25] | 5.33877757  | -5.37581383  | -1.33192937 |
| H[Z=1.25] | -7.10094134 | -2.28480043  | -1.54001993 |
| H[Z=1.25] | 5.22577019  | 4.99273545   | -2.06947660 |
| H[Z=1.25] | -8.34451593 | -0.12900059  | 1.27248858  |
| H[Z=1.25] | -7.14320674 | 1.63359233   | -1.81831376 |
| H[Z=1.25] | 1.80239715  | 6.91514004   | -2.20330676 |
| H[Z=1.25] | 7.09474695  | 0.75376053   |            |
| H[Z=0.75] | -1.71099679 | -7.28188594  | -0.96825714 |
| H[Z=0.75] | -1.05150175 | -6.24191797  | -3.00230985 |
| H[Z=0.75] | 5.68322596  | -2.26566424  | -3.29182793 |
| H[Z=0.75] | 7.03739944  | -2.11551388  | -1.34485989 |
| H[Z=0.75] | -4.46778045 | -4.32337275  | -3.13413805 |
| H[Z=0.75] | -5.13327084 | -5.36065748  | -1.10113652 |
| H[Z=0.75] | -2.95802777 | -5.18583388  | 1.67108508  |
| H[Z=0.75] | 2.26694640  | -0.34718032  | -3.42451796 |
| H[Z=0.75] | -1.13678449 | 1.56422505   | -3.55715083 |
| H[Z=0.75] | -1.09422211 | -2.33161892  | -3.27959332 |
| H[Z=0.75] | 5.97584275  | 0.02927980   | 1.29818855  |
| H[Z=0.75] | 6.99732436  | 1.80105994   | -1.62259439 |
| H[Z=0.75] | 5.64050560  | 1.64463481   | -3.56911140 |
| H[Z=0.75] | -4.55306395 | 3.48267738   | -3.69027270 |
| H[Z=0.75] | -5.24353504 | 4.78164172   | -1.82302423 |
| H[Z=0.75] | -1.86514340 | 6.77788295   | -1.96793733 |
| H[Z=0.75] | -3.07039629 | 5.04984588   | 0.94299007  |
| H[Z=0.75] | -1.17950434 | 5.47452311   | -3.83443624 |
| H[Z=0.75] | 2.31366501  | -4.24973593  | -3.13826631 |
| Element | X1  | X2  | X3  |
|---------|-----|-----|-----|
| H[Z=0.75] | 2.22892154 | 3.55675352 | -3.69270037 |
| H[Z=0.75] | -4.50607507 | -0.41968947 | -3.40360266 |
| Ga | 1.16788590 | -6.02931346 | -0.75528691 |
| Ga | 4.56094222 | -4.02927331 | -0.89427984 |
| Ga | 3.34734867 | -5.67031524 | 1.82026198 |
| Ga | -2.19717676 | -4.09697671 | -0.95224278 |
| Ga | -5.58750991 | -2.23362293 | -1.00657091 |
| Ga | -2.24749713 | -0.22687055 | -1.12658459 |
| Ga | 0.17757749 | -3.97347092 | 1.71869208 |
| Ga | 1.16260929 | -2.14572487 | -1.02209240 |
| Ga | -3.54312590 | -1.91072797 | 1.57622135 |
| Ga | 4.48136753 | -0.15732277 | -1.22959428 |
| Ga | 1.11858941 | 1.76613602 | -1.27812239 |
| Ga | 3.38838788 | -2.09647387 | 1.56695210 |
| Ga | 4.47456612 | 3.71359557 | -1.43474880 |
| Ga | 3.34424773 | 2.12020062 | 1.29500637 |
| Ga | -6.69027140 | -0.10102651 | 1.38941185 |
| Ga | -5.62735277 | 1.69023588 | -1.29861730 |
| Ga | -2.26391262 | 3.62628832 | -1.48609529 |
| Ga | -3.56536620 | 1.80506609 | 1.32735684 |
| Ga | 0.09702442 | 3.94775847 | 1.36741231 |
| Ga | 1.04782383 | 5.63010312 | -1.54462029 |
| Ga | 3.21147364 | 5.68972623 | 1.01628786 |
| P | 1.06886726 | -6.13873609 | 1.69927353 |
| P | -1.06488127 | -6.12203494 | -1.55862249 |
| P | 4.85300026 | -3.91862796 | 1.53551493 |
| P | 2.31434023 | -4.14613920 | -1.68896043 |
| P | 5.67252541 | -2.14863492 | -1.84555647 |
| P | -4.46638901 | -4.21341450 | -1.69009274 |
| P | -5.84977021 | -2.28422765 | 1.42853706 |
| P | -2.22917677 | -3.93734129 | 1.45940104 |
| P | 2.24464474 | -0.23508284 | -1.98099108 |
| P | -2.17612572 | -0.05685028 | 1.31793348 |
| P | -1.08726035 | -2.20616176 | -1.83313345 |
| P | 1.06096906 | 1.82089507 | 1.12318887 |
| P | -4.50773797 | -0.31233750 | -1.95280714 |
| P | 4.51772090 | 0.01018326 | 1.17991012 |
| P | -1.12683802 | 1.65289583 | -2.10879516 |
| P | 1.08431111 | -1.85305380 | 1.40447149 |
| P | 4.76841261 | 3.95164875 | 0.98502439 |
| P | 5.63203505 | 1.74729181 | -2.12194580 |
| P | 2.22723604 | 3.67032734 | -2.24240706 |
| P | -4.53685375 | 3.58327583 | -2.24490638 |
| P | -2.29348762 | 3.81430557 | 0.89303996 |
| P | -5.88387758 | 2.07592973 | 1.10735705 |
| P | -1.17904969 | 5.56707205 | -2.38799736 |
Py* on CdTe(111):

Total DFT Energy: -3984.403076647459 Ha

H[Z=1.50]  -8.42921687  2.30603248  -1.84213644
H[Z=1.50]  -9.70694616  0.09488896  1.75662825
H[Z=1.50]  -8.49240732  -2.37524500  -1.69396379
H[Z=1.50]  2.08019889  -8.66775263  -1.49836062
H[Z=1.50]  4.95877141  8.29449058  1.49098189
H[Z=1.50]  6.33330416  5.91470396  -1.96203366
H[Z=1.50]  6.16780402  -6.38112434  -1.57187088
H[Z=1.50]  4.73294621  -8.49963212  2.02324589
H[Z=1.50]  2.30302097  8.31595912  -2.03240206
H[Z=0.50]  -6.15293548  6.04087933  -1.70551853
H[Z=0.50]  -5.33687845  4.52432340  -4.06049985
H[Z=0.50]  -5.46299004  -4.81297424  -3.76595449
H[Z=0.50]  -5.39992360  -0.14329303  -3.88074356
H[Z=0.50]  -6.31699373  -6.15446479  -1.31905170
H[Z=0.50]  -1.25921029  6.80516895  -4.13357093
H[Z=0.50]  -2.05915987  8.32977358  -1.77935292
H[Z=0.50]  -1.38520039  -2.53231556  -3.83802219
H[Z=0.50]  2.69064439  -0.25336075  -3.91178496
H[Z=0.50]  2.75371016  4.41630547  -4.02707279
H[Z=0.50]  -1.32277737  2.13536404  -3.98676359
H[Z=0.50]  -2.28738619  -8.55281736  -1.24452426
H[Z=0.50]  2.62759937  -4.92091276  -3.73003072
H[Z=0.50]  -1.44876683  -7.20210545  -3.69071504
H[Z=0.50]  7.15925679  -0.13215321  1.78134414
H[Z=0.50]  6.76821456  2.02714591  -3.98484825
H[Z=0.50]  8.42829609  2.08982005  -1.58489459
H[Z=0.50]  -3.67079073  -6.18926406  1.97739331
H[Z=0.50]  8.36169899  -2.59823911  -1.43775378
H[Z=0.50]  6.70486592  -2.64256165  -3.83879142
H[Z=0.50]  -3.50342736  6.21560598  1.58451289
Cd  -6.64531038  2.30844205  -1.23699499
| Column 1 | Column 2 | Column 3 | Column 4 |
|---------|---------|---------|---------|
| Cd      | -6.71402154 | -2.41075640 | -1.07356597 |
| Cd      | -4.08780585  | 2.21921808  | 1.52674751  |
| Cd      | -7.79089057  | 0.08678741  | 1.66203667  |
| Cd      | -4.15866840  | -2.08616517 | 1.65871756  |
| Cd      | -2.62968173  | 4.55173932  | -1.33723747 |
| Cd      | 1.37496959   | 6.80410883  | -1.35933039 |
| Cd      | 1.33429116   | 2.20084871  | -1.24279154 |
| Cd      | 3.97266816   | 6.65393288  | 1.45624628  |
| Cd      | -2.67688702  | -0.08975664 | -1.17803279 |
| Cd      | 0.34153707   | 4.61672692  | 1.91021367  |
| Cd      | -2.74482434  | -4.73219609 | -1.03598279 |
| Cd      | 1.28554190   | -2.42515936 | -1.13124087 |
| Cd      | 3.94031748   | 2.43859537  | 1.50695828  |
| Cd      | 1.19115910   | -7.10095363 | -0.94482822 |
| Cd      | 3.87816203   | -2.59564844 | 1.63977957  |
| Cd      | 0.14180280   | -4.68227848 | 1.71901543  |
| Cd      | 3.79146893   | -6.83714560 | 1.86553796  |
| Cd      | 5.43257110   | 4.38964935  | -1.29885039 |
| Cd      | 5.34013726   | -0.19806533 | -1.19218139 |
| Cd      | 5.31646257   | -4.79657957 | -1.01365476 |
| Te      | -6.83673262  | 2.65129799  | 1.58120511  |
| Te      | -5.32400837  | 4.57458674  | -2.28914721 |
| Te      | -6.90006424  | -2.50408579 | 1.76462519  |
| Te      | -5.40430675  | -0.09938108 | -2.07289466 |
| Te      | -5.44193459  | -4.75651705 | -1.99160929 |
| Te      | -1.26513834  | 6.84682741  | -2.36446406 |
| Te      | 1.30151504   | 7.20412272  | 1.43794205  |
| Te      | -2.58643852  | 4.65549451  | 1.48174502  |
| Te      | -1.39294847  | -2.46803959 | -2.06739228 |
| Te      | 1.23010897   | 1.99969882  | 1.57303253  |
| Te      | -1.33395872  | 2.18920878  | -2.22071666 |
| Te      | 1.16427532   | -2.12445413 | 1.70683223  |
| Te      | 2.76127998   | 4.48440803  | -2.22868252 |
| Te      | -2.75122232  | -4.62292770 | 1.80451249  |
| Te      | 2.67422953   | -0.16762908 | -2.14457288 |
| Te      | -2.40073939  | 0.03368443  | 1.65926149  |
| Te      | 1.08628310   | -7.28648778 | 1.89697651  |
| Te      | -1.45709455  | -7.12527013 | -1.91765685 |
| Te      | 2.62893990   | -4.85576944 | -1.92370234 |
| Te      | 6.75755816   | 2.06865835  | -2.20966708 |
| Te      | 5.34716933   | -0.10279000 | 1.64952397  |
| Te      | 5.73185175   | 4.55013445  | 1.52860946  |
| Te      | 6.69205259   | -2.56709344 | -2.06465835 |
| Te      | 5.59149169   | -4.77156500 | 1.82288437  |
| C       | -0.11815863  | 5.87455749  | 6.32874102  |
| C       | 0.15229983   | 5.80753009  | 4.96193038  |
Py$^*$ on CuInS$_2$(112):

Total DFT Energy: -16994.595900683875 Ha

H[Z=0.25]  -3.12976999  8.10923205  1.05054985
H[Z=0.25]  -4.10288549  6.35714120  -4.02368237
H[Z=0.25]  -3.30017619  -1.55653882  -3.84091284
H[Z=0.25]  -4.86658155  -8.84584752  1.19152368
H[Z=0.25]  3.64253373  8.80650442  1.49944368
H[Z=0.25]  2.66945626  7.05440973  -3.57508878
H[Z=0.25]  -0.13818453  0.86514520  -3.64456473
H[Z=0.25]  3.47214671  -0.85926756  -3.39202006
H[Z=0.25]  0.66454772  -7.04853677  -3.46209454
H[Z=0.25]  1.90547532  -8.1490558  1.64040297
H[Z=0.25]  7.62319189  5.61595516  -0.87807614
H[Z=0.25]  6.09491260  7.6908891  1.69700461
H[Z=0.25]  6.63417818  1.56241156  -3.19627061
H[Z=0.25]  8.42411873  -2.29791106  -0.69542284
H[Z=0.25]  6.89763573  -0.21488752  1.88008146
H[Z=0.25]  7.43687244  -6.35126430  -3.01320065
H[Z=0.25]  -4.97614920  7.36644631  -2.07253506
H[Z=0.25]  -3.69847032  2.51048035  -3.54390305
H[Z=0.25]  -2.89577784  -5.40319771  -3.36083319
H[Z=0.25]  -0.50003885  4.73726016  -3.36280857
H[Z=0.25]  1.79617473  8.06371669  -1.62364120
H[Z=0.25]  3.07385347  3.20775271  -3.09501021
H[Z=0.25]  0.30266473  -3.1761533  -3.17943537
H[Z=0.25]  3.87657773  -4.70622362  -2.91193530
H[Z=0.25]  0.00452787  -8.14547297  -1.39946905
H[Z=0.25]  6.11357022  3.74987175  1.66388785
H[Z=0.25]  6.27231594  5.43423215  -2.91391072
H[Z=0.25]  6.91626277  -4.16380632  1.84695671
H[Z=0.25]  7.07498873  -2.47944496  -2.73054252
H[Z=0.25]  7.73297248  1.70153296  -1.11133344
H[Z=0.25]  6.77715044  -7.44817044  -0.95055559
H[Z=0.25]  8.53564533  -6.21214416  -0.92796623
H[Z=1.50]  -6.01255455  7.85278294  0.80477347
H[Z=1.50]  -6.35846854  0.29024268  -2.23590487

C  -0.21671099  3.52204616  4.92104364
C  -0.49890921  3.49774374  6.28651223
C  -0.44872904  4.69672908  7.00499519
H  -0.66736831  4.71052011  8.07387061
H  -0.75576425  2.5591079  6.77143276
H  -0.24177464  2.61418157  4.31928175
H  0.41463720  6.69997213  4.39202049
H  -0.06518000  6.83182309  6.84538053
N  0.10515714  4.65486036  4.27378998
| Atom | x-coordinates | y-coordinates | z-coordinates |
|------|--------------|--------------|--------------|
| H[Z=1.50] | -6.70037470 | 4.09684145 | -2.13550426 |
| H[Z=1.50] | -8.44435343 | 6.19334516 | 0.73877933 |
| H[Z=1.50] | -8.09952118 | 2.25524615 | 0.72902647 |
| H[Z=1.50] | -5.55579585 | -7.62343343 | -2.05253667 |
| H[Z=1.50] | -5.89765137 | -3.81713500 | -1.95243041 |
| H[Z=1.50] | -7.64164982 | -1.72062934 | 0.92215053 |
| H[Z=1.50] | -7.29620228 | -5.65866819 | 0.91213842 |
| H[Z=1.50] | -3.04397665 | -8.95156235 | -1.88025823 |
| H[Z=1.50] | -1.40541996 | 8.17015575 | -1.97291210 |
| H[Z=1.50] | 0.75951358 | 8.54942843 | 1.2539209 |
| H[Z=1.50] | 3.72862491 | -8.25425982 | -1.43134477 |
| H[Z=1.50] | -0.94737768 | -8.54253372 | 1.48349479 |
| H[Z=1.50] | 5.36723257 | 8.86715979 | -1.52399472 |
| H[Z=1.50] | 5.82494602 | -7.84526234 | 1.93239062 |
| Cu | -3.11608932 | 4.72362251 | 1.11185546 |
| Cu | -5.18919611 | 4.36988789 | -1.44756495 |
| Cu | -2.62482556 | 0.74013000 | 1.18410172 |
| Cu | -6.82313430 | 6.42246051 | 0.76700901 |
| Cu | -2.30681713 | -3.27725080 | 1.24861844 |
| Cu | -4.40484646 | -3.48145268 | -1.28608967 |
| Cu | -1.77893572 | -7.21358202 | 1.29880412 |
| Cu | -6.03842765 | -1.60451424 | 0.92982921 |
| Cu | 3.62205674 | 5.47069074 | 1.58907526 |
| Cu | 1.55474460 | 5.08365841 | -0.96697200 |
| Cu | 4.09228430 | 1.39800108 | 1.59842868 |
| Cu | 1.52018303 | 2.69168373 | -1.18588849 |
| Cu | 0.00449643 | 7.08303552 | 1.20854020 |
| Cu | 4.44533654 | -2.45393099 | 1.68244056 |
| Cu | 2.33642974 | -2.71660707 | -0.82525971 |
| Cu | 4.96215496 | -6.52347663 | 1.72846633 |
| Cu | -0.75442806 | -5.13293014 | -0.97480501 |
| Cu | 0.72535322 | -0.88445152 | 1.45053740 |
| Cu | 5.00552668 | 3.41987762 | -0.74020854 |
| Cu | 5.84158238 | -4.41473150 | -0.57331926 |
| In | -6.37341032 | 2.44570175 | 0.76349216 |
| In | -5.57411817 | -5.46277375 | 0.97027478 |
| In | -4.67600304 | 0.42326265 | -1.64814752 |
| In | -3.90063764 | -7.45670619 | -1.46559757 |
| In | -2.06166556 | 6.58649993 | -1.40688878 |
| In | 0.41300134 | 3.11003644 | 1.64622137 |
| In | -1.25646671 | -1.19674589 | -1.26110060 |
| In | 1.29512872 | -4.78796130 | 1.66396586 |
| In | 1.96109699 | 1.07015794 | -1.17073333 |
| In | 2.74476389 | -6.77916996 | -1.03108892 |
| In | 4.69731870 | 7.28812128 | -0.91372803 |
| In | 5.54691359 | -0.46749746 | -0.81770382 |
\begin{verbatim}
S   -5.42410011  4.60229475  0.96841293
S   -4.96887978  0.45237726  0.84129345
S   -3.72842518  2.59388457 -2.15163972
S   -4.24185668  6.26593820 -2.49708261
S   -4.58367237 -3.33087260  1.14254740
S   -4.10160638 -7.45006281  0.98990182
S   -2.93711663 -5.30003485 -1.97029584
S   -3.47767624 -1.57318840 -2.30657212
S   -0.29524352  0.88582939 -2.10710368
S   1.36730562  5.27569613  1.35923554
S   -0.58150167  4.73507987 -1.97751283
S   1.80876260  1.12210259  1.27399709
S   2.89540724  3.25714363 -1.72058792
S   2.54842111  6.97839856 -2.05598948
S   -2.25442672  6.84577612  0.98397106
S   -1.91598483  2.83766354  1.11651640
S   0.48243975 -6.95477538 -1.93339381
S   2.19097943 -2.61081260  1.55117730
S   0.19343951 -3.12728420 -1.78768662
S   2.66720552 -6.80196774  1.42602012
S   3.71832205 -4.61983155 -1.54727776
S   3.33914002 -0.83363962 -1.85674771
S   -1.48981735 -1.18138386  1.17910216
S   -1.05223011 -5.12162225  1.42013431
S   6.44720192  1.67358815 -1.65916808
S   6.18083897  5.42723392 -1.52099033
S   4.56694315  7.56737007  1.45480758
S   4.75968902  3.53916499  1.62174973
S   7.23951405 -6.22735182 -1.44799535
S   6.97415970 -2.43952194 -1.34103693
S   5.41456659 -0.42251099  1.60374175
S   5.56902417 -4.39206266  1.80303220
C   0.08059447  3.78874759  6.07538501
C   0.27584928  3.90868435  4.70407597
C   0.12094221  1.60376079  4.41275277
C  -0.07820641  1.40483859  5.77368210
C  -0.09890468  2.51596895  6.62019512
H   -0.25362468  2.39125015  7.68707122
H   -0.21124955  0.39891819  6.15520309
H   0.14012270  0.77324121  3.71327253
H   0.41638409  4.87370281  4.22610787
H   0.06986894  4.67736396  6.69604801
N   0.29696104  2.83475555  3.88805877
DHP* on GaP(111):
Total DFT Energy: -8503.781029602360 Ha
\end{verbatim}
| H[Z=1.25]     | -3.11185828 | -6.44580967 | -2.10776926 |
| H[Z=1.25]     | -1.41705092 | -7.99346424 |  0.78116079 |
| H[Z=1.25]     |  0.75829139 | -7.11937510 | -2.11546307 |
| H[Z=1.25]     | -6.69208575 |  3.29699371 | -1.53631429 |
| H[Z=1.25]     |  7.42034554 |  0.84155227 | -1.56389227 |
| H[Z=1.25]     | -6.39969337 |  5.40266961 |  1.55961700 |
| H[Z=1.25]     | -4.17410808 |  6.30518275 | -1.32745363 |
| H[Z=1.25]     |  6.06756424 |  4.52346658 | -1.34820094 |
| H[Z=1.25]     |  7.69244418 |  2.89264691 |  1.53539798 |
| H[Z=0.75]     | -5.85679852 | -4.02428473 | -1.76093768 |
| H[Z=0.75]     | -4.56946271 | -3.43564348 | -3.67146262 |
| H[Z=0.75]     |  3.14101119 | -4.77703452 | -3.68656955 |
| H[Z=0.75]     |  4.15991264 | -5.76576539 | -1.78116870 |
| H[Z=0.75]     | -5.91945592 |  0.23853628 | -3.45492393 |
| H[Z=0.75]     | -7.20955757 | -0.34407737 | -1.54448417 |
| H[Z=0.75]     | -5.59606168 | -1.94144041 |  1.15598257 |
| H[Z=0.75]     |  1.79102556 | -1.10280135 | -3.47064905 |
| H[Z=0.75]     |  0.44600221 |  2.55796129 | -2.5576558 |
| H[Z=0.75]     | -2.05712273 | -0.43336647 | -3.46258379 |
| H[Z=0.75]     |  4.59304068 | -3.76693321 |  1.13941646 |
| H[Z=0.75]     |  6.67834856 | -2.76042973 | -1.57204887 |
| H[Z=0.75]     |  5.65335118 | -1.77475751 | -3.47787813 |
| H[Z=0.75]     | -0.90397980 |  6.23222024 | -3.04008988 |
| H[Z=0.75]     | -0.69263975 |  7.44300628 | -1.00538891 |
| H[Z=0.75]     |  3.17624216 |  6.77128422 | -1.01254586 |
| H[Z=0.75]     |  0.98000489 |  5.91799500 |  1.70051225 |
| H[Z=0.75]     |  2.95834204 |  5.56023744 | -3.04688881 |
| H[Z=0.75]     | -0.71376279 | -4.10287369 | -3.66980740 |
| H[Z=0.75]     |  4.30231375 |  1.89059536 | -3.25361545 |
| H[Z=0.75]     | -3.40846373 |  3.23206663 | -3.23881875 |
| Ga            | -2.85862353 | -4.98129784 | -1.46723789 |
| Ga            |  1.01194280 | -5.64738719 | -1.47579070 |
| Ga            | -1.10227012 | -6.41157218 |  1.06640497 |
| Ga            | -4.15330872 | -1.33028062 | -1.30870806 |
| Ga            | -5.35577023 |  2.28539595 | -1.06006136 |
| Ga            | -1.69573562 |  1.65092915 | -1.05742533 |
| Ga            | -2.39024124 | -3.08137360 |  1.28646668 |
| Ga            | -0.34348958 | -2.02928346 | -1.27314366 |
| Ga            | -3.91597876 |  0.89662319 |  1.48100206 |
| Ga            |  3.45748157 | -2.67397953 | -1.31343032 |
| Ga            |  2.14514588 |  0.96218352 | -1.05937853 |
| Ga            |  1.18944928 | -3.77455220 |  1.44516399 |
| Ga            |  5.97915950 |  0.28015418 | -1.09837448 |
| Ga            |  3.95505835 | -0.52654745 |  1.45649530 |
| Ga            | -5.13801499 |  4.33322294 |  1.63438935 |
| Ga            | -3.01389119 |  5.30678476 | -0.84185698 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ga      | 0.79191776 | 4.60797209 | -0.91195819 |
| Ga      | -1.55006614 | 3.74815570 | 1.69068456 |
| Ga      | 2.65122645 | 2.97475838 | 1.66094967 |
| Ga      | 4.62701248 | 3.97561713 | -0.86240102 |
| Ga      | 6.16848439 | 2.30278437 | 1.62986173 |
| P       | -3.13278250 | -5.27114487 | 0.93283175 |
| P       | -4.57518024 | -3.51208815 | -2.22023704 |
| P       | 1.17965329 | -6.05803018 | 0.87532680 |
| P       | -0.73072729 | -4.19657877 | -2.22253577 |
| P       | 3.12258702 | -4.85724752 | -2.24079857 |
| P       | -5.91823780 | 0.13840313 | -2.00631715 |
| P       | -5.89406045 | 2.14246371 | 1.36244395 |
| P       | -4.21238503 | -1.46559885 | 1.10162327 |
| P       | 1.76375709 | -1.18816051 | -2.02764312 |
| P       | -1.65776956 | 1.45225588 | 1.38428570 |
| P       | -2.04894735 | -0.51591212 | -2.01731179 |
| P       | 2.01006320 | 0.76020016 | 1.37579119 |
| P       | -3.42748894 | 3.15091290 | -1.78645147 |
| P       | 3.44445931 | -2.85508269 | 1.08721265 |
| P       | 0.42899735 | 2.45370171 | -1.80853474 |
| P       | -0.33220667 | -2.03378824 | 1.10714514 |
| P       | 6.23061837 | -0.00378089 | 1.32783110 |
| P       | 5.61719535 | -1.87549745 | -2.02912052 |
| P       | 4.28195294 | 1.80443853 | -1.80113446 |
| P       | -0.91681535 | 6.13526479 | -1.59453082 |
| P       | 0.75683026 | 4.48552957 | 1.49883345 |
| P       | -3.10687989 | 5.49558807 | 1.59707252 |
| P       | 2.92725605 | 5.46592072 | -1.60031256 |
| P       | 4.69861788 | 4.10718517 | 1.58437624 |
| H       | 1.94450569 | -4.06487750 | 4.01572732 |
| H       | -1.47336981 | -6.29203063 | 4.38583577 |
| H       | 0.96735896 | -6.13128852 | 3.96336274 |
| C       | 0.32457950 | -5.26282657 | 4.01796011 |
| C       | -1.00161181 | -5.32809322 | 4.23031920 |
| N       | 0.96696569 | -4.01508749 | 3.73096641 |
| H       | 0.64305166 | -2.78745305 | 5.43741163 |
| H       | 0.70878417 | -1.93770484 | 3.87592998 |
| H       | -1.72810351 | -1.97317736 | 4.34714174 |
| C       | -1.17348260 | -2.90500040 | 4.30178460 |
| C       | 0.33194172 | -2.82934158 | 4.38181698 |
| C       | -1.79513084 | -4.09787284 | 4.25596973 |
| H       | -2.87893712 | -4.16391492 | 4.24984349 |

*DHP* on CdTe(111):

Total DFT Energy: -3985.584190890424 Ha

H[Z=1.50] -8.63901193 -1.69558945 -1.68015914
| Element | X               | Y               | Z               |
|---------|----------------|----------------|----------------|
| H[Z=1.50] | -8.74672317 | -4.25430034 | 1.91372190 |
| H[Z=1.50] | -6.60963948 | -5.91582947 | -1.57235711 |
| H[Z=1.50] | 5.65986901  | -6.84386729 | -1.55708025 |
| H[Z=1.50] | 0.73059719  | 9.61819109  | 1.54769282 |
| H[Z=1.50] | 2.97052436  | 8.10838404  | -1.94248907 |
| H[Z=1.50] | 8.30124312  | -2.97631698 | -1.65863111 |
| H[Z=1.50] | 8.01174948  | -5.52173008 | 1.93434098 |
| H[Z=1.50] | -1.70776757 | 8.46426973  | -1.94382218 |
| H[Z=0.50] | -8.26153344 | 2.66143959  | -1.53749653 |
| H[Z=0.50] | -6.88994991 | 1.67322481  | -3.91516364 |
| H[Z=0.50] | -2.84237849 | -6.74492336 | -3.70116724 |
| H[Z=0.50] | -4.86594546 | -2.53485562 | -3.77567990 |
| H[Z=0.50] | -2.97437234 | -8.33273502 | -1.25661415 |
| H[Z=0.50] | -4.25548697 | 5.53085401  | -4.01645133 |
| H[Z=0.50] | -5.61626318 | 6.53360775  | -1.63917604 |
| H[Z=0.50] | -0.20746233 | -2.88705166 | -3.80145804 |
| H[Z=0.50] | 2.42629048  | 0.96856806  | -3.90319144 |
| H[Z=0.50] | 0.40226920  | 5.17840430  | -3.97819808 |
| H[Z=0.50] | -2.23149844 | 1.32075927  | -3.90092499 |
| H[Z=0.50] | 1.70218094  | -8.68600546 | -1.25084894 |
| H[Z=0.50] | 4.45029572  | -3.23946074 | -3.76170935 |
| H[Z=0.50] | 1.81652823  | -7.09713734 | -3.69443278 |
| H[Z=0.50] | 6.45568188  | 3.05154618  | 1.73775127  |
| H[Z=0.50] | 5.06075251  | 4.82619685  | -4.00447810 |
| H[Z=0.50] | 6.55413496  | 5.61497672  | -1.62367642 |
| H[Z=0.50] | -0.54195568 | -7.19448158 | 2.00823861  |
| H[Z=0.50] | 8.58358657  | 1.38753827  | -1.51717812 |
| H[Z=0.50] | 7.08519503  | 0.61630060  | -3.8945825  |
| H[Z=0.50] | -5.91942669 | 3.98867232  | 1.72269722  |
| Cd      | -7.01388509  | -0.86946369 | -1.08058615 |
| Cd      | -4.97205367  | -5.13406500 | -0.97245711 |
| Cd      | -4.66703483  | 0.19678751  | 1.68492829 |
| Cd      | -6.97401770  | -3.40779226 | 1.79358818  |
| Cd      | -2.84293210  | -3.79664935 | 1.74599011 |
| Cd      | -4.39263996  | 2.90630429  | -1.13992781 |
| Cd      | -1.85105741  | 6.66139940  | -1.2856634 |
| Cd      | 0.18315974   | 2.55228579  | -1.23013464 |
| Cd      | 0.54196485   | 7.61164322  | 1.69187267 |
| Cd      | -2.40265183  | -1.26892051 | -1.07471587 |
| Cd      | -1.63615699  | 4.35762928  | 1.99660913 |
| Cd      | -0.40534278  | -5.44430333 | -0.99145701 |
| Cd      | 2.18773416   | -1.60884560 | -1.07891447 |
| Cd      | 2.31785322   | 3.95465335  | 1.75455908 |
| Cd      | 4.15403036   | -5.82154672 | -0.96744002 |
| Cd      | 4.66110706   | -0.55433881 | 1.66668772 |
| Cd      | 2.22012830   | -4.17202305 | 1.74285889 |
| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Cd      | 6.38195546 | -4.41958994  | 1.82524287 |
| Cd      | 2.84816961  | 6.32141776   | -1.25619766 |
| Cd      | 4.79361024  | 2.20855528   | -1.15129403 |
| Cd      | 6.81518169  | -1.91715108  | -1.06832828 |
| Te      | -7.31642766 | -0.68902656  | 1.75592440  |
| Te      | -6.85120514 | 1.75118923   | -2.13302932 |
| Te      | -5.09870524 | -5.40759347  | 1.87071778  |
| Te      | -4.85841700 | -2.48504202  | -1.97248622 |
| Te      | -2.81576270 | -6.69244737  | -1.92836894 |
| Te      | -4.26786097 | 5.55123192   | -2.24896509 |
| Te      | -2.13174893 | 7.05939968   | 1.48850378  |
| Te      | -4.36453068 | 3.04714189   | 1.70055654  |
| Te      | -0.20954973 | -2.81874697  | -2.03157749 |
| Te      | 0.14755817  | 2.28735242   | 1.56245596  |
| Te      | -2.23746685 | 1.35935357   | -2.14885200 |
| Te      | 2.03339581  | -1.42339169  | 1.76900715  |
| Te      | 0.40858336  | 5.23233916   | -2.19418445 |
| Te      | -0.41215372 | -5.38871033  | 1.85709009  |
| Te      | 2.41542153  | 1.01951426   | -2.14084821 |
| Te      | -2.2229131 | -1.11224022  | 1.77138736  |
| Te      | 4.21754142  | -6.09919649  | 1.87958307  |
| Te      | 1.79030565  | -7.04051227  | -1.92257776 |
| Te      | 4.43757323  | -3.18258862  | -1.96003045 |
| Te      | 5.06579207  | 4.85415591   | -2.23030462 |
| Te      | 4.79426625  | 2.31699318   | 1.69349712  |
| Te      | 3.09356190  | 6.61382211   | 1.54445698  |
| Te      | 7.05544837  | 0.69690860   | -2.11885840 |
| Te      | 7.15497291  | -1.79113184  | 1.76921337  |
| H       | -2.05532065 | 4.60320748   | 4.80165261  |
| H       | 1.06721121  | 7.28048599   | 4.78280899  |
| H       | -1.36051992 | 6.78135138   | 4.62695786  |
| C       | -0.60866305 | 6.00234998   | 4.63941974  |
| C       | 0.71589501  | 6.25728334   | 4.70451184  |
| N       | -1.09992810 | 4.68994649   | 4.46213099  |
| H       | -0.43659139 | 3.49516300   | 6.09609479  |
| H       | -0.56062250 | 2.66123227   | 4.53507776  |
| H       | 1.88936663  | 3.02456142   | 4.77529372  |
| C       | 1.21064493  | 3.87236118   | 4.77450657  |
| C       | -0.25534735 | 3.59562631   | 5.01271440  |
| C       | 1.66005891  | 5.13890402   | 4.66844855  |
| H       | 2.71986484  | 5.34264917   | 4.55371269  |

*DHP* on CuInS₂(112):

Total DFT Energy: -16995.773655796373 Ha

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| H[Z=0.25] | -3.11549344 | 8.13274702 | 1.11355345 |
| H[Z=0.25] | -4.08543545 | 6.42037527 | -3.97482646 |
| Z       | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| 0.25    | -3.29276225 | -1.49546129 | -3.85119755 |
| 0.25    | -4.87354493  | -8.82072615  | 1.12421051  |
| 0.25    | 3.65721500   | 8.81811819   | 1.57480155  |
| 0.25    | 2.68729442   | 7.10574484   | -3.51387861 |
| 0.25    | -0.12796925  | 0.92070458   | -3.63319509 |
| 0.25    | 3.47994536   | -0.81009122  | -3.38995051 |
| 0.25    | 0.66472411   | -6.99513170  | -3.50986549 |
| 0.25    | 1.89889625   | -8.13568495  | 1.58544127  |
| 0.25    | 7.63638765   | 5.64069431   | -0.82266539 |
| 0.25    | 6.10798440   | 7.70616790   | 1.76652889  |
| 0.25    | 6.64477880   | 1.60607423   | -3.17254669 |
| 0.25    | 8.42727518   | -2.27532532  | -0.69915598 |
| 0.25    | 6.90066764   | -0.20996740  | 1.89046288  |
| 0.25    | 7.43743354   | -6.30976043  | -3.04861733 |
| 0.75    | -4.95949836  | 7.41595952   | -2.01700043 |
| 0.75    | -3.68630961  | 2.56986808   | -3.52379060 |
| 0.75    | -2.89365664  | -5.34615077  | -3.39986137 |
| 0.75    | -0.48530321  | 4.79102344   | -3.32248033 |
| 0.75    | 1.81321028   | 8.10132869   | -1.55575233 |
| 0.75    | 3.08639890   | 3.25505725   | -3.06254351 |
| 0.75    | 0.30736016   | -3.12511314  | -3.19825000 |
| 0.75    | 3.87908327   | -4.66107795  | -2.93861144 |
| 0.75    | 0.00116370   | -8.10683833  | -1.45630393 |
| 0.75    | 6.12176380   | 3.75729479   | 1.70350298  |
| 0.75    | 6.28743591   | 5.47609417   | -2.86123046 |
| 0.75    | 6.91441683   | -4.15854206  | 1.82743122  |
| 0.75    | 7.08006887   | -2.43974397  | -2.73700290 |
| 0.75    | 7.74154440   | 1.72801757   | -1.08546698 |
| 0.75    | 6.77417100   | -7.42143752  | -0.99503567 |
| 0.75    | 8.53417743   | -6.18782057  | -0.96124042 |
| 1.50    | -5.99833383  | 7.88177716   | 0.86282569  |
| 1.50    | -6.35044681  | 0.34293321   | -2.23543908 |
| 1.50    | -6.68772277  | 4.14908702   | -2.10655023 |
| 1.50    | -8.43212429  | 6.22593310   | 0.78171387  |
| 1.50    | -8.09218152  | 2.28759239   | 0.74247657  |
| 1.50    | -5.55781395  | -7.57290393  | -2.11121153 |
| 1.50    | -5.89503933  | -3.76704827  | -1.98261923 |
| 1.50    | -7.63946089  | -1.69020482  | 0.90594219  |
| 1.50    | -7.29890248  | -5.62848185  | 0.86644676  |
| 1.50    | -3.04785321  | -8.90544396  | -1.94637648 |
| 1.50    | -1.38787903  | 8.21441968   | -1.90755483 |
| 1.50    | 0.77411794   | 8.56651963   | 1.32435355  |
| 1.50    | 3.72515409   | -8.22004316  | -1.48510822 |
| 1.50    | -0.95427706  | -8.52454066  | 1.42257078  |
| 1.50    | 5.38515776   | 8.89952194   | -1.44628487 |
| 1.50    | 5.81843135   | -7.83917049  | 1.88382088  |
|   |   |   |   |
|---|---|---|---|
| Cu | -3.09909152 | 4.73723510 | 1.14706305 |
| Cu | -5.17354738 | 4.41200846 | -1.42244667 |
| Cu | -2.61055509 | 0.75503669 | 1.20006862 |
| Cu | -6.80978686 | 6.45140572 | 0.81255170 |
| Cu | -2.31467739 | -3.27181492 | 1.21554187 |
| Cu | -4.40420434 | -3.43627642 | -1.31112713 |
| Cu | -1.78671644 | -7.19637741 | 1.24555199 |
| Cu | -6.03622805 | -1.56655533 | 0.91282966 |
| Cu | 3.62914265 | 5.48277693 | 1.64269067 |
| Cu | 1.57396040 | 5.11667276 | -0.92741341 |
| Cu | 4.09191302 | 1.41170480 | 1.63764956 |
| Cu | -1.49875276 | 2.73142976 | -1.15404933 |
| Cu | 0.01630971 | 7.10057935 | 1.26398907 |
| Cu | 4.43655230 | -2.44263253 | 1.67645779 |
| Cu | 2.33378782 | -2.67239131 | -0.83296070 |
| Cu | 4.95912475 | -6.51236700 | 1.68994771 |
| Cu | -0.75395549 | -5.09921811 | -1.01188974 |
| Cu | 0.70859082 | -0.85068652 | 1.47259856 |
| Cu | 5.01335025 | 3.44399309 | -0.70019527 |
| Cu | 5.83998393 | -4.38261695 | -0.59728741 |
| In | -6.36545811 | 2.47946514 | 0.78049451 |
| In | -5.57589090 | -5.43620363 | 0.92779380 |
| In | -4.66584167 | 0.47058694 | -1.64159020 |
| In | -3.90331914 | -7.41226459 | -1.52413249 |
| In | -2.04815660 | 6.62593749 | -1.35201394 |
| In | 0.43334840 | 3.12001368 | 1.69391259 |
| In | -1.24949618 | -1.16027650 | -1.27157962 |
| In | 1.29416624 | -4.76551865 | 1.63072320 |
| In | 1.96252091 | 1.10748180 | -1.14859781 |
| In | 2.74559105 | -6.74440443 | -1.07193953 |
| In | 4.71105392 | 7.31585701 | -0.84645271 |
| In | 5.54598275 | -0.43559390 | -0.79993599 |
| S  | -5.40888662 | 4.63085575 | 0.99469756 |
| S  | -4.96041199 | 0.48444560 | 0.84877005 |
| S  | -3.71303391 | 2.64152350 | -2.12960628 |
| S  | -4.22504576 | 6.31976872 | -2.45217724 |
| S  | -4.59136146 | -3.30482607 | 1.11752179 |
| S  | -4.10707001 | -7.42532412 | 0.92950022 |
| S  | -2.93841418 | -5.25328381 | -2.00813214 |
| S  | -3.47431537 | -1.52362782 | -2.31580560 |
| S  | -0.28717407 | 0.92987973 | -2.10002053 |
| S  | 1.37929422 | 5.29435613 | 1.39127802 |
| S  | -0.56642035 | 4.78068783 | -1.93718063 |
| S  | 1.81749119 | 1.14064877 | 1.28669138 |
| S  | 2.90744884 | 3.29410260 | -1.68912092 |
| S  | 2.56690434 | 7.02226799 | -2.00006892 |
|        |        |        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| S      | -2.24400329 | 6.86606966 | 1.03994844 |
| S      | -1.89428004  | 2.85270144  | 1.14766093 |
| S      | 0.48390657   | -6.91350686 | -1.97878700 |
| S      | 2.18086841   | -2.58430922 | 1.53891417 |
| S      | 0.19746509   | -3.08878399 | -1.80687468 |
| S      | 2.66169229   | -6.78432645 | 1.38498322 |
| S      | 3.71740844   | -4.58087347 | -1.57413333 |
| S      | 3.34288117   | -0.79084477 | -1.85194506 |
| S      | -1.49869559  | -1.17767667 | 1.15527957 |
| S      | -1.05196129  | -5.10895295 | 1.38209385 |
| S      | 6.45533195   | 1.70619871  | -1.63218403 |
| S      | 6.19402651   | 5.45955622  | -1.46818221 |
| S      | 4.58160596   | 7.58025828  | 1.52370567 |
| S      | 4.76758135   | 3.55067837  | 1.65936419 |
| S      | 7.23810344   | -6.19685851 | -1.48220056 |
| S      | 6.97682887   | -2.40388343 | -1.34649266 |
| S      | 5.41467024   | -0.41204649 | 1.62173887 |
| S      | 5.5659973    | -4.3808592  | 1.77790294 |
| H      | 0.52470611   | 4.06829703  | 4.27222675 |
| H      | 2.34113825   | 0.45888379  | 5.04175492 |
| H      | 2.47529910   | 2.93416555  | 4.67636643 |
| C      | 1.56940988   | 2.35487324  | 4.54750155 |
| C      | 1.47512916   | 1.02582588  | 4.71919319 |
| N      | 0.43835798   | 3.08105403  | 4.02889713 |
| H      | -0.93601070  | 2.76132188  | 5.61852665 |
| H      | -1.66177946  | 3.08664751  | 4.02248878 |
| H      | -1.86388384  | 0.61542216  | 4.01370331 |
| C      | -0.91313509  | 1.07020290  | 4.27173542 |
| C      | -0.86219059  | 2.55410613  | 4.53932930 |
| C      | 0.21787492   | 0.35073366  | 4.39436055 |
| H      | 0.22098247   | -0.72422698 | 4.23680193 |

\(2-\text{PyH}^+\) on GaP(111):

Total DFT Energy: -8503.301904727501 Ha

| H[Z=1.25] |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        | 1.17439210 | -7.56844824 | -1.15949550 |
| H[Z=1.25] | 3.37225046 | -7.50649936 | 1.80345988 |
| H[Z=1.25] | 4.75056774 | -5.94787860 | -1.28806380 |
| H[Z=1.25] | -7.28371455 | -1.54010940 | -1.59120130 |
| H[Z=1.25] | 5.75633782 | 4.36990529 | -2.05963568 |
| H[Z=1.25] | -8.30675455 | 0.74775801 | 1.20579829 |
| H[Z=1.25] | -6.90318659 | 2.35905286 | -1.88235043 |
| H[Z=1.25] | 2.56011883 | 6.64817430 | -2.22305954 |
| H[Z=1.25] | 4.74718571 | 6.60220694 | 0.74840067 |
| H[Z=0.75] | -2.46531854 | -7.08466770 | -0.96653209 |
| H[Z=0.75] | -1.68484115 | -6.12950184 | -2.99935052 |
| H[Z=0.75] | 5.43964023 | -2.90039839 | -3.25552942 |
|    | x       | y       | z       |
|----|---------|---------|---------|
| P  | -2.6393 | -3.6880 | 1.4538  |
| P  | 2.2256  | -0.5016 | -1.9707 |
| P  | -2.1208 | 0.1804  | 1.2759  |
| P  | -1.2965 | -2.1079 | -1.8425 |
| P  | 1.2169  | 1.7104  | 1.0978  |
| P  | -4.4922 | 0.1461  | -1.9920 |
| P  | 4.4924  | -0.4946 | 1.2005  |
| P  | -0.9185 | 1.7341  | -2.1357 |
| P  | 0.8950  | -2.0548 | 1.4379  |
| P  | 5.1448  | 3.3960  | 1.0046  |
| P  | 5.8113  | 1.0970  | -2.0978 |
| P  | 2.6385  | 3.3790  | -2.2505 |
| P  | -4.0988 | 4.0179  | -2.2970 |
| P  | -1.8553 | 4.0279  | 0.8442  |
| P  | -5.6068 | 2.6737  | 1.0639  |
| P  | -0.5489 | 5.6280  | -2.4260 |
| P  | 1.5867  | 5.9319  | 0.7947  |
| C  | -0.5597 | 3.2763  | 5.6472  |
| C  | -0.4956 | 3.0331  | 4.1548  |
| C  | 1.6258  | 4.1185  | 4.1729  |
| C  | 1.7981  | 3.8313  | 5.5075  |
| C  | 0.5996  | 3.5651  | 6.2814  |
| H  | 0.6293  | 3.6864  | 7.3632  |
| H  | 2.7491  | 4.0304  | 5.9895  |
| H  | 2.4374  | 4.5677  | 3.5977  |
| H  | -1.4778 | 3.1358  | 3.6801  |
| H  | -1.5029 | 3.1658  | 6.1750  |
| N  | 0.4427  | 3.9754  | 3.5095  |
| H  | -0.1629 | 1.9910  | 3.9517  |

2-PyH* on CdTe(111):

Total DFT Energy: -3985.09415106 Ha

| Z   | x       | y       | z       |
|-----|---------|---------|---------|
| 1.50| -8.3143 | 2.6513  | -1.8587 |
| 1.50| -9.6908 | 0.4986  | 1.7389  |
| 1.50| -8.5726 | -2.0231 | -1.7068 |
| 1.50| 1.7286  | -8.7498 | -1.4824 |
| 1.50| 5.3038  | 8.0806  | 1.4994  |
| 1.50| 6.5857  | 5.6426  | -1.9485 |
| 1.50| 5.9079  | -6.6353 | -1.5486 |
| 1.50| 4.3783  | -8.6890 | 2.0450  |
| 1.50| 2.6590  | 8.2094  | -2.0298 |
| 0.50| -5.8849 | 6.2883  | -1.7200 |
| 0.50| -5.1275 | 4.7370  | -4.0719 |
| 0.50| -5.6426 | -4.5866 | -3.7700 |
| 0.50| -5.3850 | 0.0762  | -3.8885 |
| 0.50| -6.5571 | -5.8892 | -1.3239 |
|        |        |        |        |        |
|--------|--------|--------|--------|--------|
| H[Z=0.50] | -0.95832388 | 6.84620431 | -4.13776705 |
| H[Z=0.50] | -1.69933559  | 8.40491697  | -1.78659763 |
| H[Z=0.50] | -1.47334199  | -2.47768080 | -3.83484417 |
| H[Z=0.50] | 2.69394224   | -0.37033504 | -3.90134682 |
| H[Z=0.50] | 2.95148881   | 4.29255739  | -4.02032242 |
| H[Z=0.50] | -1.21644655  | 2.18322294  | -3.98727303 |
| H[Z=0.50] | -2.63094266  | -8.45306732 | -1.23843717 |
| H[Z=0.50] | 2.43635789   | -5.03105529 | -3.71590671 |
| H[Z=0.50] | -1.73146451  | -7.14064674 | -3.68385037 |
| H[Z=0.50] | 7.15117168   | -0.42994547 | 1.80167512  |
| H[Z=0.50] | 6.86301338   | 1.73849008  | -3.96714742 |
| H[Z=0.50] | 8.51897236   | 1.73423542  | -1.56353387 |
| H[Z=0.50] | -3.92191036  | -6.03106738 | 1.97843458  |
| H[Z=0.50] | 8.25706209   | -2.94685802 | -1.41269821 |
| H[Z=0.50] | 6.60511466   | -2.92440379 | -3.81740351 |
| H[Z=0.50] | -3.23772180  | 6.35573622  | 1.57575757  |
| Cd     | -6.53329085  | 2.58635905  | -1.24193849 |
| Cd     | -6.79457375  | -2.11841048 | -1.09727698 |
| Cd     | -3.96587098  | 2.42451933  | 1.54587892  |
| Cd     | -7.77679300  | 0.39780197  | 1.65812678  |
| Cd     | -4.22415707  | -1.91512891 | 1.65166727  |
| Cd     | -2.41673584  | 4.67232965  | -1.33301988 |
| Cd     | 1.68084845   | 6.72951573  | -1.32821323 |
| Cd     | 1.44206854   | 2.13433736  | -1.24118933 |
| Cd     | 4.24511081   | 6.48454733  | 1.49184432  |
| Cd     | -2.65663252  | 0.03006010  | -1.18646574 |
| Cd     | 0.59592981   | 4.61754758  | 2.11482842  |
| Cd     | -2.93545775  | -4.62120407 | -1.04788559 |
| Cd     | 1.19376425   | -2.48830948 | -1.13427312 |
| Cd     | 4.03187809   | 2.25176971  | 1.52557873  |
| Cd     | 0.90399552   | -7.14760772 | -0.93430275 |
| Cd     | 3.76244644   | -2.74571713 | 1.66845026  |
| Cd     | -0.04965181  | -4.67106420 | 1.73114563  |
| Cd     | 3.51179480   | -6.98810874 | 1.89193421  |
| Cd     | 5.62692758   | 4.15999223  | -1.28315210 |
| Cd     | 5.34945537   | -0.42879708 | -1.18615726 |
| Cd     | 5.11576784   | -5.02057885 | -0.99083972 |
| Te     | -6.71312302  | 2.91847362  | 1.58103585  |
| Te     | -5.11201130  | 4.79001266  | -2.29910522 |
| Te     | -6.98421268  | -2.22689468 | 1.74540880  |
| Te     | -5.38596935  | 0.13364174  | -2.08655248 |
| Te     | -5.62776580  | -4.52681971 | -1.99769156 |
| Te     | -0.95111044  | 6.89707637  | -2.36827066 |
| Te     | 1.60554095   | 7.16236875  | 1.45688382  |
| Te     | -2.36756387  | 4.77168822  | 1.48046786  |
| Te     | -1.48545804  | -2.41120324 | -2.06677063 |
2-PyH* on CuInS₂(112):
Total DFT Energy: -16995.293230243748 Ha

H[Z=0.25]  -3.18792511  8.10214490  1.05336199
H[Z=0.25]  -4.17520701  6.34987223  -4.01807070
H[Z=0.25]  -3.32041512  -1.55865829  -3.84907616
H[Z=0.25]  -4.81430102  -8.86398064  1.18218957
H[Z=0.25]   3.58191957  8.84271005  1.46908930
H[Z=0.25]   2.59465731   7.09043402  -3.60264375
H[Z=0.25]  -0.17320563   0.88320950  -3.66563333
H[Z=0.25]   3.44942874  -0.81809427  -3.43334991
H[Z=0.25]   0.68160463  -7.02532248  -3.49693822
H[Z=0.25]   1.95527889  -8.12374763  1.59790326
H[Z=0.25]   7.57109961   5.68085061  -0.93232128
H[Z=0.25]   6.04235298   7.75095902  1.65296586
H[Z=0.25]   6.59667508  1.62376962  -3.25050593
H[Z=0.25]   8.42410662  -2.22787753  -0.76343422
H[Z=0.25]   6.89715908  -0.15786820  1.82226730
H[Z=0.25]   7.45145030  -6.28475723  -3.08121087
| Atom [Z=0.75] | X       | Y       | Z       |
|--------------|---------|---------|---------|
| H            | -5.04515031 | 7.35116369 | -2.06132064 |
| H            | -3.74350772  | 2.50533815  | -3.54506383 |
| H            | -2.88873425  | -5.40319091 | -3.37576886 |
| H            | -0.55867570  | 4.75256017  | -3.37729737 |
| H            | 1.72469461   | 8.09172685  | -1.64559332 |
| H            | 3.02633703   | 3.24590329  | -3.12933753 |
| H            | 0.29611232   | -3.15626660 | -3.20769948 |
| H            | 3.88114423   | -4.66292383 | -2.96003803 |
| H            | 0.03907929   | -8.12897967 | -1.43237503 |
| H            | 6.08638752   | 3.80198795  | 1.61489503  |
| H            | 6.21120201   | 5.49282513  | -2.96156658 |
| H            | 6.94116105   | -4.10654111 | 1.78418900  |
| H            | 7.06595728   | -2.41570345 | -2.79197317 |
| H            | 7.70502207   | 1.76750352  | -1.17094488 |
| H            | 6.80922272   | -7.38838246 | -1.01662957 |
| H            | 8.55977740   | -6.14102507 | -1.00135246 |
| H            | -6.07019064  | 7.82733196  | 0.82175407  |
| H            | -6.38247516  | 0.26635972  | -2.22645416 |
| H            | -6.74848641  | 4.07054206  | -2.11965218 |
| H            | -8.49150639  | 6.15226514  | 0.76593376  |
| H            | -8.12126255  | 2.21649571  | 0.74960175  |
| H            | -5.52772000  | -7.64216788 | -2.05686075 |
| H            | -5.89368014  | -3.83828516 | -1.95035373 |
| H            | -7.63671836  | -1.75656064 | 0.93552964  |
| H            | -7.26586095  | -5.69226562 | 0.91893538  |
| H            | -3.00654886  | -8.95421240 | -1.89883657 |
| H            | -1.47923816  | 8.17785417  | -1.97864628 |
| H            | 0.69940395   | 8.56726824  | 1.23776667  |
| H            | 3.76359457   | -8.21361519 | -1.48309112 |
| H            | -0.89572168  | -8.53564934 | 1.45484314  |
| H            | 5.29093709   | 8.91815309  | -1.56289742 |
| H            | 5.87412300   | -7.79508518 | 1.87057245  |
| Cu           | -3.14761033  | 4.70945611  | 1.10602901  |
| Cu           | -5.22993585  | 4.34415938  | -1.44264901 |
| Cu           | -2.63470872  | 0.73511434  | 1.17864043  |
| Cu           | -6.87114052  | 6.39060032  | 0.78577961  |
| Cu           | -2.28451922  | -3.27975966 | 1.22925169  |
| Cu           | -4.39721694  | -3.49765828 | -1.29187765 |
| Cu           | -1.74097610  | -7.21367135 | 1.27686811  |
| Cu           | -6.03371585  | -1.63565809 | 0.93553098  |
| Cu           | 3.57518596   | 5.50260552  | 1.56740357  |
| Cu           | 1.50257711   | 5.09677953  | -0.98253753 |
| Cu           | 4.06105793   | 1.43628198  | 1.57928986  |
| Cu           | -1.52878137  | 2.70084699  | -1.16601611 |
| Cu           | -0.04514722  | 7.09129804  | 1.19223691  |
| Cu           | 4.45524770   | -2.40773527 | 1.63776108  |
| Metal | X1 | Y1 | Z1 | X2 | Y2 | Z2 | X3 | Y3 | Z3 |
|-------|----|----|----|----|----|----|----|----|----|
| Cu    | 2.33930535 | -2.67472381 | -0.85815123 |
| Cu    | 4.99883715 | -6.47733241 | 1.67231618 |
| Cu    | -0.73389374 | -5.12185946 | -1.00154539 |
| Cu    | 0.72989167 | -0.84928913 | 1.42794786 |
| Cu    | 4.9594224 | 3.46383067 | -0.77294613 |
| Cu    | 5.8584628 | -4.35178472 | -0.63168764 |
| In    | -6.39288755 | 2.41735234 | 0.77243247 |
| In    | -5.54335896 | -5.4801865 | 0.97245115 |
| In    | -4.69509936 | 0.40857842 | -1.64751189 |
| In    | -3.87495297 | -7.46851204 | -1.47260163 |
| In    | -2.12117192 | 6.58770688 | -1.40802326 |
| In    | 0.38654187 | 3.12841848 | 1.72068906 |
| In    | -1.25983400 | -1.18484347 | -1.27753314 |
| In    | 1.32455906 | -4.76531679 | 1.62392551 |
| In    | 1.93623553 | 1.10184470 | -1.19760669 |
| In    | 2.77444874 | -6.74487473 | -1.07655970 |
| In    | 4.63052423 | 7.3302469 | -0.94580953 |
| In    | 5.52819769 | -0.40902427 | -0.85861321 |
| S     | -5.46095030 | 4.58066310 | 0.97834068 |
| S     | -4.97958780 | 0.42913010 | 0.84154543 |
| S     | -3.75651853 | 2.58243261 | -2.15057782 |
| S     | -4.30640462 | 6.25532696 | -2.49052122 |
| S     | -4.56316521 | -3.34869838 | 1.14195082 |
| S     | -4.06213497 | -7.46675376 | 0.98085586 |
| S     | -2.92239285 | -5.30841343 | -1.98431351 |
| S     | -3.48794807 | -1.58088926 | -2.31185982 |
| S     | -0.32551176 | 0.90339560 | -2.13224822 |
| S     | 1.32888015 | 5.29803929 | 1.32718581 |
| S     | -0.63350363 | 4.74835086 | -1.99135148 |
| S     | 1.79863809 | 1.14577208 | 1.22289602 |
| S     | 2.85450972 | 3.29414042 | -1.75794832 |
| S     | 2.48138795 | 7.01159925 | -2.08314436 |
| S     | -2.30886812 | 6.84561425 | 0.98166290 |
| S     | -1.93103005 | 2.83544778 | 1.13064851 |
| S     | 0.50804106 | -6.93486548 | -1.96787601 |
| S     | 2.20014437 | -2.58182659 | 1.52002913 |
| S     | 0.19545110 | -3.10936904 | -1.81489737 |
| S     | 2.70418400 | -6.77493018 | 1.38079656 |
| S     | 3.73220117 | -4.57917555 | -1.59414850 |
| S     | 3.32739112 | -0.79365125 | -1.90222973 |
| S     | -1.48473702 | -1.17988187 | 1.15964323 |
| S     | -1.02197243 | -5.11908564 | 1.39322417 |
| S     | 6.41625646 | 1.73404007 | -1.71093877 |
| S     | 6.12534880 | 5.48527059 | -1.56798454 |
| S     | 4.51518226 | 7.61058253 | 1.42309605 |
| S     | 4.73381571 | 3.58189380 | 1.58482753 |
2-PyH* + CO₂ Transition State on GaP(111):

Total DFT Energy: -8691.911829261793 Ha, 726.0 i cm⁻¹

**H[Z=1.25]**
- 2.32340933 -7.27085147  -1.30829128
- 4.54371097  -6.85537336   1.60823308
- 5.58440706  -5.08816919  -1.50258861
- 7.01244663  -2.70458076  -1.53639956
- 4.87489039  5.25662572  -2.24342071
- 8.33609929  -0.61882690  1.29242328
- 2.40378326  3.66240766  3.90085579
- 1.18769994  1.54340902  3.92594432
- 0.97114303  1.08619863  6.36790237
- 0.53021863  2.75183053  3.82077625
- 0.33333098  0.64142892  3.85408048

S 7.26135368 -6.1636916  -1.51486651
S 6.97393564 -2.37003218  -1.40143493
S 5.41621133  -0.37040792   1.56326335
S 5.59456257  -4.34177775   1.74440493
C 0.11162993  1.45174995  5.81228481
C 0.16002003  1.53486734  4.30399963
C 1.74433712  2.95908568  4.41135373
C 2.10583576  2.42193246  5.62729476
C 1.05197709  1.79976782  6.40988811
H 1.1774792  1.70898748  7.48788775
H 3.05659454  2.68920273  6.07649455
H 2.40378326  3.66240766  3.90085579
H -1.18769994  1.54340902  3.92594432
H -0.97114303  1.08619863  6.36790237
N 0.53021863  2.75183053  3.82077625
H 0.33333098  0.64142892  3.85408048

**H[Z=0.75]**
- 1.34714754  6.98228322  -2.32937571
- 3.57442122  7.28940087  0.59583307
- 1.34075429  -7.38900511  -1.03921368
- 0.77012589  -6.31621425  -3.08193314
- 5.72491694  -1.96545390  -3.46904169
- 7.09591775  -1.73720231  -1.54113840
- 4.29029110  -4.59336146  -3.16897326
- 4.86831279  -5.66433577  -1.12417291
- 2.66713361  -5.36364145  1.61653333
- 2.20392962  -0.24375085  -3.55414510
- 1.30391629  1.47201945  3.63953488
- 1.03782297  -2.41412388  -3.36023387
- 5.95132978  0.34763340  1.11587165
- 6.83036325  2.17031189  -1.81941669
- 5.45738294  1.93565088  -3.74728841
- 4.82408052  3.19487241  -3.72465382
- 5.56046458  4.45518833  -1.84872402
- 2.30256811  6.63836560  -2.04195499
- 3.36769052  4.84878549  0.88630618
- 1.57161339  5.37410982  -3.91777660

42
| Element | x | y | z |
|---------|---|---|---|
| H[Z=0.75] | 2.47544203 | -4.13714625 | -3.26696900 |
| H[Z=0.75] | 1.94151042 | 3.65207260 | -3.82350598 |
| H[Z=0.75] | -4.55355445 | -0.69868633 | -3.43745619 |
| Ga | 1.46976760 | -5.97392690 | -0.86510352 |
| Ga | 4.73666481 | -3.78452061 | -1.06310620 |
| Ga | 3.65985863 | -5.49180099 | 1.67844917 |
| Ga | -2.00144156 | -4.24029004 | -1.01066210 |
| Ga | -5.49285568 | -2.56649672 | -1.03810873 |
| Ga | -2.28079113 | -0.38031727 | -1.19237503 |
| Ga | 0.39853482 | -3.97906199 | 1.62511827 |
| Ga | 1.22564237 | -2.09979009 | -1.14042658 |
| Ga | -3.43963620 | -2.13956318 | 1.53506423 |
| Ga | 4.42840024 | 0.07335405 | -1.38721489 |
| Ga | 0.96946469 | 1.82242441 | -1.39958463 |
| Ga | 3.47201440 | -1.91059374 | 1.43134981 |
| Ga | 4.20557621 | 3.94143178 | -1.60007394 |
| Ga | 3.21419290 | 2.29008144 | 1.15632580 |
| Ga | -6.68572785 | -0.49398367 | 1.39524809 |
| Ga | -5.76180750 | 1.34694677 | -1.31330907 |
| Ga | -2.51862275 | 3.46909957 | -1.54291963 |
| Ga | -3.64665520 | 1.58035928 | 1.27220104 |
| Ga | -0.12684027 | 3.98148503 | 1.37787196 |
| Ga | 0.67333787 | 5.66071185 | -1.65225266 |
| Ga | 2.86273553 | 5.84774569 | 0.87202052 |
| P | 1.40986807 | -6.08883551 | 1.59308251 |
| P | -0.76523577 | -6.19625052 | -1.63672254 |
| P | 5.04603251 | -3.64779520 | 1.37002473 |
| P | 2.48675670 | -4.02869395 | -1.81838124 |
| P | 5.72754562 | -1.84347140 | -2.02298333 |
| P | -4.27040477 | -4.48355585 | -1.72289026 |
| P | -5.72488776 | -2.63059284 | 1.40118373 |
| P | -2.00767760 | -4.07985647 | 1.40273985 |
| P | 2.18822021 | -0.12874266 | -2.10947369 |
| P | -2.16976682 | -0.22357236 | 1.25147943 |
| P | -1.02631760 | -2.29060441 | -1.91582898 |
| P | 0.94917501 | 1.93083985 | 0.97284258 |
| P | -4.54414588 | -0.58884136 | -1.98669175 |
| P | 4.49238235 | 0.24803835 | 1.01920919 |
| P | -1.28012926 | 1.56359579 | -2.19098736 |
| P | 1.15181088 | -1.80951180 | 1.28386871 |
| P | 4.52403872 | 4.20590345 | 0.82256388 |
| P | 5.46233397 | 2.04050014 | -2.29873854 |
| P | 1.95512360 | 3.77488619 | -2.37812041 |
| P | -4.79637350 | 3.29535745 | -2.27918402 |
| P | -2.51115607 | 3.66448436 | 0.83078967 |
| P | -5.98666618 | 1.71702030 | 1.09938526 |
2-PyH$^+ + \text{CO}_2$ Transition State on CdTe(111):

| Atom | $Z=1.50$ | $Z=0.50$ |
|------|----------|----------|
| P    | -1.55835154 5.46448522 | -2.47033907 |
| P    | 0.57389247 6.13497823 | 0.70711072 |
| C    | -1.21712796 3.08322358 | 5.46608480 |
| C    | -0.77230247 2.85391346 | 4.07387767 |
| C    | 0.42739148 4.90969808 | 4.20043124 |
| C    | 0.33834396 4.93923733 | 5.57439229 |
| C    | -0.60521498 4.05480248 | 6.19653706 |
| H    | -0.86621771 4.20169594 | 7.24221050 |
| H    | 0.85080836 5.70528711 | 6.13983947 |
| H    | 0.98211304 5.67122728 | 3.65557824 |
| H    | -1.51098090 2.35591013 | 3.43899111 |
| H    | -1.95962604 2.41766532 | 5.89500464 |
| N    | -0.22327441 4.00411440 | 3.42721305 |
| H    | 0.08389410 1.99765086 | 4.09420291 |
| O    | -0.09890733 -0.19369765 | 4.29090958 |
| C    | 0.81358464 0.58270374 | 4.20707892 |
| O    | 1.99141611 0.82220011 | 4.21149170 |

Total DFT Energy: $-4173.707626196976$ Ha, 583.2 $i$ cm$^{-1}$
| Substance | x (Å) | y (Å) | z (Å) |
|-----------|-------|-------|-------|
| H[Z=0.50] | -3.92200000 | -6.03100000 | 1.97800000 |
| H[Z=0.50] | 8.25700000 | -2.94700000 | -1.41300000 |
| H[Z=0.50] | 6.60500000 | -2.92400000 | -3.81700000 |
| H[Z=0.50] | -3.23800000 | 6.35600000 | 1.57600000 |
| Cd | -6.51175396 | 2.58922853 | -1.23868246 |
| Cd | -6.77385047 | -2.11923657 | -1.09833281 |
| Cd | -3.95088330 | 2.42273439 | 1.56685466 |
| Cd | -7.74509458 | 0.39328167 | 1.67096276 |
| Cd | -4.21988839 | -1.92839908 | 1.67935664 |
| Cd | -2.41480449 | 4.6686516 | -1.34849320 |
| Cd | 1.66395554 | 6.71464299 | -1.30716989 |
| Cd | 1.44894005 | 2.13523795 | -1.27653730 |
| Cd | 4.24051160 | 6.44424098 | 1.52341990 |
| Cd | -2.64769781 | 0.02882849 | -1.17433249 |
| Cd | 0.55839111 | 4.56457823 | 2.10639733 |
| Cd | -2.93118661 | -4.61349669 | -1.04698763 |
| Cd | 1.19584960 | -2.48335550 | -1.11799311 |
| Cd | 3.98689067 | 2.26885064 | 1.58681457 |
| Cd | 0.89281890 | -7.13095782 | -0.93321221 |
| Cd | 3.77512723 | -2.71923181 | 1.69799083 |
| Cd | -0.05164438 | -4.67260342 | 1.75127489 |
| Cd | 3.49685937 | -6.95763612 | 1.90156397 |
| Cd | 5.62313366 | 4.13723476 | -1.27437045 |
| Cd | 5.33945683 | -0.41821620 | -1.15796290 |
| Cd | 5.11362144 | -4.99585658 | -0.99339617 |
| Te | -6.69948223 | 2.91884111 | 1.58775204 |
| Te | -5.10961104 | 4.79642000 | -2.30204896 |
| Te | -6.98142864 | -2.23644535 | 1.74839453 |
| Te | -5.37401039 | 0.13492669 | -2.08518639 |
| Te | -5.62310884 | -4.53139001 | -1.99855558 |
| Te | -0.95358767 | 6.89933116 | -2.36886986 |
| Te | 1.59825381 | 7.10875262 | 1.49288687 |
| Te | -2.36822907 | 4.77343153 | 1.46664196 |
| Te | -1.47900789 | -2.40733823 | -2.06664549 |
| Te | 1.27445570 | 1.91814224 | 1.51003116 |
| Te | -1.22793657 | 2.24801769 | -2.23193325 |
| Te | 1.07284029 | -2.16265851 | 1.72265162 |
| Te | 2.96677450 | 4.36799917 | -2.22683928 |
| Te | -2.93218759 | -4.51230594 | 1.79730970 |
| Te | 2.68644222 | -0.29489653 | -2.14109462 |
| Te | -2.39116823 | 0.12953766 | 1.67074678 |
| Te | 0.78240210 | -7.31906659 | 1.91332138 |
| Te | -1.74783588 | -7.06292011 | -1.91422538 |
| Te | 2.43227005 | -4.96048763 | -1.91138340 |
| Te | 6.85537504 | 1.77368437 | -2.19405090 |
| Te | 5.34087599 | -0.30905579 | 1.68532457 |
2-PyH* + CO2 Transition State on CuInS2(112):
Total DFT Energy: -17183.903738000088 Ha, 733.1 i cm⁻¹

H[Z=0.25]  -3.18626551  8.12507234  1.06924746
H[Z=0.25]  -4.22583844  6.40134682  -4.00093485
H[Z=0.25]  -3.38911773 -1.51048714  -3.88016435
H[Z=0.25]  -4.85353085 -8.83730382  1.12774934
H[Z=0.25]   3.58921844  8.84728272  1.42450988
H[Z=0.25]   2.54963450  7.12256230  -3.64667645
H[Z=0.25]  -0.23440422  0.92279688  -3.71476775
H[Z=0.25]   3.38536628 -0.78827531  -3.52489141
H[Z=0.25]   0.60231900 -6.98038098  -3.59399218
H[Z=0.25]   1.92095165 -8.11609098  1.48301720
H[Z=0.25]   7.54725626  5.68774153 -1.03035774
H[Z=0.25]   6.04810825  7.74830975  1.57954024
H[Z=0.25]   6.54107123  1.64501135  -3.36050428
H[Z=0.25]   8.38197707 -2.22408751 -0.90956819
H[Z=0.25]   6.88482896 -0.16352422  1.70031074
H[Z=0.25]   7.37680049 -6.26682524  -3.23872531
H[Z=0.75]  -5.07467384  7.39450861 -2.03069268
H[Z=0.75]  -3.8000891  2.55294161 -3.55155065
H[Z=0.75]  -2.96328669 -5.35789237  -3.43077508
H[Z=0.75]  -0.60792667  4.79221159  -3.40249811
H[Z=0.75]   1.70080161  8.11672307  -1.67642922
H[Z=0.75]   2.97547604  3.27515099  -3.19628825
H[Z=0.75]   0.22879404 -3.11962337  -3.28172761
H[Z=0.75]   3.81219575 -4.63668298  -3.07551774
H[Z=0.75]  -0.02378214  8.10095010  -1.52858474
|         |          |          |          |          |
|---------|----------|----------|----------|----------|
| H[Z=0.75] | 6.08183599 | 3.79946006 | 1.52111237 |          |
| H[Z=0.75] | 6.16754626 | 5.51342607 | -3.04824071 |          |
| H[Z=0.75] | 6.91855670 | -4.11237390 | 1.64188287 |          |
| H[Z=0.75] | 7.00427648 | -2.39841298 | -2.92647027 |          |
| H[Z=0.75] | 7.66918580 | 1.77569308 | -1.29044752 |          |
| H[Z=0.75] | 6.75169330 | -7.37873563 | -1.17432228 |          |
| H[Z=0.75] | 8.50588871 | -6.13614596 | -1.16867807 |          |
| H[Z=1.50] | -6.07101192 | 7.85834492 | 0.86431121 |          |
| H[Z=1.50] | -6.43095485 | 0.31375505 | -2.21885391 |          |
| H[Z=1.50] | -6.78638167 | 4.11905323 | -2.09052451 |          |
| H[Z=1.50] | -8.49762920 | 6.18961796 | 0.82289001 |          |
| H[Z=1.50] | -8.13667544 | 2.25285137 | 0.78341297 |          |
| H[Z=1.50] | -5.59523158 | -7.59707647 | -2.09806882 |          |
| H[Z=1.50] | -5.95065140 | -3.79278336 | -1.96831348 |          |
| H[Z=1.50] | -7.66089898 | -1.72222110 | 0.94466054 |          |
| H[Z=1.50] | -7.29995322 | -5.65798261 | 0.90418855 |          |
| H[Z=1.50] | -3.07614500 | -8.91606367 | -1.97073263 |          |
| H[Z=1.50] | -1.50592422 | 8.21230155 | -1.97846397 |          |
| H[Z=1.50] | 0.70347057  | 8.57955777  | 1.21957808 |          |
| H[Z=1.50] | 3.70033740  | -8.19485574 | -1.61548381 |          |
| H[Z=1.50] | -0.93230315 | -8.52034051 | 1.36508641 |          |
| H[Z=1.50] | 5.26949003  | 8.93351194  | -1.62320562 |          |
| H[Z=1.50] | 5.84318182  | -7.79813014 | 1.72034982 |          |
| Cu      | -3.16638168 | 4.73724839 | 1.09655444 |          |
| Cu      | -5.26330127 | 4.38507043 | -1.42364384 |          |
| Cu      | -2.63994370 | 0.76925536 | 1.15365353 |          |
| Cu      | -6.87807605 | 6.42672621 | 0.82973069 |          |
| Cu      | -2.31661107 | -3.25472847 | 1.19358291 |          |
| Cu      | -4.45181346 | -3.46028998 | -1.31114506 |          |
| Cu      | -1.76980503 | -7.19171381 | 1.20486954 |          |
| Cu      | -6.05744718 | -1.59996669 | 0.93330508 |          |
| Cu      | 3.58151852  | 5.50951047 | 1.49925894 |          |
| Cu      | 1.48065508  | 5.11974224 | -1.02607122 |          |
| Cu      | 4.04040132  | 1.44100906 | 1.49120013 |          |
| Cu      | -1.56070664 | 2.72693522 | -1.22004143 |          |
| Cu      | -0.04409007 | 7.10220387 | 1.17522860 |          |
| Cu      | 4.43686725  | -2.39790677 | 1.54461141 |          |
| Cu      | 2.30885954  | -2.66502423 | -0.96634764 |          |
| Cu      | 4.96797733  | -6.47476699 | 1.54043352 |          |
| Cu      | -0.78810560 | -5.09261778 | -1.07074724 |          |
| Cu      | 0.70620174  | -0.86165132 | 1.35612847 |          |
| Cu      | 4.93305954  | 3.47323188 | -0.86104716 |          |
| Cu      | 5.81627345  | -4.33887277 | -0.75870368 |          |
| In      | -6.40776802 | 2.44764832 | 0.79639237 |          |
| In      | -5.57223104 | -5.46279541 | 0.96409682 |          |
| In      | -4.73743578 | 0.44743126 | -1.65619778 |          |
| In         | -3.93906883 | -7.42709906 | -1.53229281 |
| In         | -2.14746812 | 6.62119314  | -1.41112297 |
| In         | 0.38465502  | 3.13692060  | 1.65139231  |
| In         | -1.30725342 | -1.16782583 | -1.32341883 |
| In         | 1.29511042  | -4.75226296 | 1.52361984  |
| In         | 1.89239935  | 1.12015642  | -1.26265715 |
| In         | 2.71987089  | -6.72523442 | -1.19179616 |
| In         | 4.61118147  | 7.34769884  | -1.01384934 |
| In         | 5.48951024  | -0.39999676 | -0.96678118 |
| S          | -5.47393292 | 4.60928525  | 1.00365069  |
| S          | -4.99158268 | 0.45778469  | 0.82889892  |
| S          | -3.80183867 | 2.62186573  | -2.15802169 |
| S          | -4.34489645 | 6.29759497  | -2.47130722 |
| S          | -4.59500312 | -3.32441734 | 1.12627025  |
| S          | -4.09405645 | -7.44453078 | 0.91649951  |
| S          | -2.98677233 | -5.26790352 | -2.03816043 |
| S          | -3.54571284 | -1.54408222 | -2.33868145 |
| S          | -0.37494928 | 0.92226012  | -2.17955825 |
| S          | 1.32981311  | 5.30635178  | 1.28906911  |
| S          | -0.66502115 | 4.78373062  | -2.01704213 |
| S          | 1.77041060  | 1.14785462  | 1.16869342  |
| S          | 2.81485051  | 3.31185917  | -1.82150536 |
| S          | 2.44860373  | 7.03484275  | -2.12429682 |
| S          | -2.31025353 | 6.86617543  | 0.98203842  |
| S          | -1.94068092 | 2.86727435  | 1.07435163  |
| S          | 0.44276728  | -6.90503467 | -2.06207889 |
| S          | 2.18774263  | -2.57809164 | 1.39526883  |
| S          | 0.14634481  | -3.08411135 | -1.88741991 |
| S          | 2.66747514  | -6.76513202 | 1.26652852  |
| S          | 3.68451972  | -4.56179279 | -1.70802919 |
| S          | 3.27782139  | -0.76751207 | -1.99410086 |
| S          | -1.51205310 | -1.15698035 | 1.11457832  |
| S          | -1.05576461 | -5.09590194 | 1.33084355  |
| S          | 6.37481053  | 1.74608588  | -1.81600931 |
| S          | 6.09669484  | 5.40839411  | -1.65442017 |
| S          | 4.51813416  | 7.61377927  | 1.35796423  |
| S          | 4.72812063  | 3.58189816  | 1.49903043  |
| S          | 7.20247260  | -6.15190192 | -1.66832372 |
| S          | 6.92696904  | -2.35912420 | -1.53487215 |
| S          | 5.40050414  | -0.36320144 | 1.45384626  |
| S          | 5.56964428  | -4.33958562 | 1.61688613  |
| C          | -0.48915735 | 1.73193048  | 5.76282733  |
| C          | -0.11589402 | 1.64411749  | 4.33333119  |
| C          | 1.20671002  | 3.59835705  | 4.62195043  |
| C          | 1.20384218  | 3.45204877  | 5.99194793  |
| C          | 0.22851142  | 2.56624696  | 6.56396296  |
$H^* + CO_2$ Transition State on GaP(111):
Total DFT Energy: -8443.497804313205 Ha, 740.5 i cm$^{-1}$

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 0.03249424 | 2.60844713 | 7.63306741 |
| H       | 1.80724799 | 4.10533714 | 6.61191103 |
| H       | 1.77126222 | 4.39518100 | 4.14060749 |
| H       | -0.89771033 | 1.23946628 | 3.68125625 |
| H       | -1.25959873 | 1.07259745 | 6.15037047 |
| N       | 0.44069700  | 2.84450041 | 3.78618764 |
| H       | 0.72302223 | 0.77823466 | 4.22081532 |
| O       | 0.68280000  | -1.40447592 | 4.56495880 |
| C       | 1.54571791  | -0.58609557 | 4.39429898 |
| O       | 2.70283325  | -0.27142256 | 4.34945569 |
| Ga      | -5.43002045 | -2.47009662 | -0.93525343 |
| Ga      | -2.73972277 | -5.33041016 | -0.90540685 |
| Ga      | -4.79399986 | -4.49144055 | 1.69212149 |
| Element | x          | y          | z          |
|---------|------------|------------|------------|
| Ga      | -4.29856848| 1.23925570 | -1.06265669|
| Ga      | -3.22997836| 4.96539847 | -1.02967234|
| Ga      | -0.51983335| 2.16530903 | -1.04796259|
| Ga      | -3.80378510| -1.04283379| 1.63981891 |
| Ga      | -1.63235874| -1.59164832| 0.97177319 |
| Ga      | -2.73588027| 3.07591565 | 1.68401322 |
| Ga      | 1.02461510 | -4.40739823| -0.98645476|
| Ga      | 2.16205273 | -0.67555327| -0.97820000|
| Ga      | -1.27206168| -3.73980968| 1.66851613 |
| Ga      | 4.80688508 | -3.53637170| -0.95002599|
| Ga      | 2.80359649 | -2.73351847| 1.63606974 |
| Ga      | -1.62456617| 6.49538949 | 1.48561075 |
| Ga      | 0.60148066 | 5.85335222 | -1.00577601|
| Ga      | 3.22864734 | 3.05645534 | -1.04471768|
| Ga      | 1.23641784 | 3.92209385 | 2.97047133 |
| Ga      | 3.93352198 | 0.87381867 | 1.58598710 |
| Ga      | 5.93816588 | 0.24907945 | -1.02264811|
| Ga      | 6.29323819 | -1.88895782| 1.58414468 |
| P       | -5.72181120| -2.36754334| 1.50052417 |
| P       | -5.97060305| -0.31228087| -1.77798940|
| P       | -2.72699972| -5.56305097| 1.54103894 |
| P       | -3.28736761| -3.15901007| 1.73490409 |
| P       | -0.60656758| -6.00058523| -1.71627194|
| P       | -4.85217950| 3.42897758 | -1.83345218|
| P       | -3.59928578| 5.23551067 | 1.37942126 |
| P       | -4.30384042| 1.30366386 | 1.33398439 |
| P       | 0.52345085 | -2.23494476| -1.77106394|
| P       | -0.42662351| 2.69908595 | 1.34193926 |
| P       | -2.15115137| 0.58788382 | -1.79718342|
| P       | 2.04943125 | -0.53449759| 1.45824830 |
| P       | -1.06155272| 4.36204966 | -1.84630031|
| P       | 1.04519883 | -4.38880586| 1.43659565 |
| P       | 1.63035615 | 1.49070728 | -1.82826062|
| P       | -1.51875527| -1.43002898| 1.46278653 |
| P       | 4.91304481 | -3.75215326| 1.48848536 |
| P       | 3.19323103 | -5.10190166| -1.73929453|
| P       | 4.33038146 | -1.34966327| -1.78155116|
| P       | 2.74290617 | 5.24311534 | -1.87826820|
| P       | 3.21938834 | 3.14053656 | 1.33625079 |
| P       | 0.61925606 | 5.96365311 | 1.36778393 |
| P       | 5.41604633 | 2.40915047 | -1.84919475|
| P       | 6.22596811 | 0.41848218 | 1.41188168 |
| H       | -0.70824044| 1.35151402 | 2.30982254 |
| C       | -1.07203235| 1.16585956 | 3.56977164 |
| O       | -0.26828160| 0.46104129 | 4.14879073 |
| O       | -2.09638273| 1.81139085 | 3.81252624 |
**DHP$^*$ + CO$_2$ Transition State on GaP(111):**

Total DFT Energy: -8692.364675051274 Ha, 933.3 i cm$^{-1}$

| Atom | Z=1.25 | Z=0.75 |
|------|--------|--------|
| H    |        |        |
|      | -3.11185828 | -6.44580967 |
|      | -1.41705092 | -7.99346424 |
|      | 0.75829139 | -7.11937510 |
|      | -6.69208575 | 3.29699371 |
|      | 7.42034554 | 0.84155227 |
|      | -6.39969337 | 5.40266961 |
|      | -4.17410808 | 6.30518275 |
|      | 6.06756424 | 4.52346658 |
|      | 7.69244418 | 2.89264691 |
|      | -5.85679852 | -4.02428473 |
|      | -4.56946271 | -3.43564348 |
|      | 3.14101119 | -4.77703452 |
|      | 4.15991264 | -5.76576539 |
|      | -5.91945592 | 0.23853628 |
|      | -7.20955757 | -0.34407737 |
|      | -5.59606168 | -1.94144041 |
|      | 1.79102556 | -1.10280135 |
|      | 0.44600221 | 2.55796129 |
|      | -2.05712273 | -0.43336647 |
|      | 4.59304068 | -3.76693321 |
|      | 6.67834856 | -2.76042973 |
|      | 5.65335118 | -1.77475751 |
|      | -0.90397980 | 6.23222024 |
|      | -0.69263975 | 7.44300628 |
|      | 3.17624216 | 6.77128422 |
|      | 0.98000489 | 5.91799500 |
|      | 2.95834204 | 5.56023744 |
|      | -0.71376279 | -4.10287369 |
|      | 4.30231375 | 1.89059536 |
|      | -3.40846373 | 3.23206663 |

| Atom |        |
|------|--------|
| Ga   | -2.86696644 |
| Ga   | 1.01475639 |
| Ga   | -1.12263025 |
| Ga   | -4.16193553 |
| Ga   | -5.53720234 |
| Ga   | -1.69633495 |
| Ga   | -2.39679870 |
| Ga   | -0.35797906 |
| Ga   | -3.91847696 |
| Ga   | 3.46887220 |
| Ga   | 2.14227739 |
| Ga   | 1.23364221 |
| Ga   | 5.97980632 |

Ga   | -4.98001971 |
Ga   | -5.65523798 |
Ga   | -6.40894967 |
Ga   | -1.32469003 |
Ga   | 2.28911346 |
Ga   | 1.65745538 |
Ga   | -3.06756083 |
Ga   | -2.01900394 |
Ga   | 0.90320491 |
Ga   | -2.65757221 |
Ga   | 0.96540345 |
Ga   | -3.70586643 |
Ga   | 0.28795705 |
| Ga    | 3.95813978 | -0.49384715 | 1.45943862 |
| Ga    | -5.14022093 | 4.33573491 | 1.63527103 |
| Ga    | -3.01525391 | 5.30890518 | -0.84116392 |
| Ga    | 0.79060968 | 4.60960496 | -0.91052097 |
| Ga    | -1.55208428 | 3.75060306 | 1.69531482 |
| Ga    | 2.64928337 | 2.97863150 | 1.66397986 |
| Ga    | 4.62755260 | 3.97857055 | -0.86253679 |
| Ga    | 6.17024301 | 2.31067162 | 1.63129317 |
| P     | -3.14184598 | -5.25780114 | 0.94127122 |
| P     | -4.57809630 | -3.50735173 | -2.22044497 |
| P     | 1.16978494 | -6.02208629 | 0.93009113 |
| P     | -0.73347051 | -4.19765329 | -2.22319345 |
| P     | 3.12634590 | -4.85201094 | -2.23859587 |
| P     | -5.92133135 | 0.14321193 | -2.00676169 |
| P     | -5.89704810 | 2.14509678 | 1.36319581 |
| P     | -4.21466383 | -1.45767398 | 1.09916573 |
| P     | 1.75936226 | -1.18434381 | -2.02869078 |
| P     | -1.66052270 | 1.45381541 | 1.39067330 |
| P     | -2.05937989 | -0.50628360 | -2.01807822 |
| P     | 2.00272942 | 0.76416060 | 1.38035969 |
| P     | -3.42862821 | 3.15303155 | -1.78583676 |
| P     | 3.47569772 | -2.82416583 | 1.06833194 |
| P     | 0.42743875 | 2.45560398 | -1.80796421 |
| P     | -0.33734466 | -2.00862591 | 1.10189827 |
| P     | 6.23340928 | 0.00374590 | 1.32817331 |
| P     | 5.62570779 | -1.86797501 | -2.03201926 |
| P     | 4.27968013 | 1.80751250 | -1.80098394 |
| P     | -0.91773700 | 6.13560858 | -1.59437456 |
| P     | 0.75477842 | 4.48636058 | 1.50005435 |
| P     | -3.10870232 | 5.49717404 | 1.59759958 |
| P     | 2.92619146 | 5.46638153 | -1.60021662 |
| P     | 4.69655786 | 4.11086775 | 1.58439834 |
| H     | 1.95683077 | -2.50784565 | 4.14813085 |
| H     | -0.72283831 | -5.64805289 | 5.01362801 |
| H     | 1.61196441 | -4.82232615 | 4.60877809 |
| C     | 0.74512557 | -4.17333927 | 4.58665860 |
| C     | -0.53396618 | -4.60587755 | 4.79006250 |
| N     | 0.99474054 | -2.86908558 | 4.25503624 |
| H     | 0.23835287 | -1.37364024 | 5.60902874 |
| H     | 0.25204288 | -0.96870949 | 3.85113666 |
| H     | -2.14207021 | -1.62323450 | 4.26158022 |
| C     | -1.35023548 | -2.34896379 | 4.40444879 |
| C     | 0.02865035 | -1.86693196 | 4.42530993 |
| C     | -1.60864224 | -3.66923682 | 4.62487140 |
| H     | -2.63417725 | -4.02430970 | 4.64528700 |
| C     | 1.07570908 | -0.93309107 | 6.64868151 |
### $H^*$ on GaP(111):

**Total DFT Energy: -8254.921005496215 Ha**

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| O    | 2.19933019 | -1.30661508 | 6.37648087 |
| O    | 0.40014948  | -0.32879760  | 7.45650440  |

| Atom | x     | y     | z     |
|------|-------|-------|-------|
| Ga   | -5.42901191 | -2.47331011 | -0.93704606 |
| Ga   | -2.73961381 | -5.32979049 | -0.90840673 |
| Ga   | -4.78993859 | -4.49910571 | 1.68922328 |
| Ga   | -4.29499291 | 1.23509711  | -1.05337018 |
| Ga   | -3.20925196 | 4.96758364  | -1.04901411 |
| Ga   | -0.52468908 | 2.18556925  | -1.04940719 |
| Ga   | -3.80621297 | -1.06093720 | 1.64211673 |
| Ga   | -1.62869739 | -1.58026112 | -0.96384824 |
| Ga   | -2.69733823 | 3.03817318  | 1.59529179  |
| Ga   | 1.02660731  | -4.40812798 | -0.98760480 |
| Ga   | 2.15699239  | -0.67064562 | 0.97303049  |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ga      | -1.26819209 | -3.75887398 | 1.67089118 |
| Ga      | 4.80830619  | -3.53415314 | -0.95092640 |
| Ga      | 2.82164661  | -2.74650426 | 1.63202061 |
| Ga      | -1.51890773 | 6.51177115  | 1.49443115 |
| Ga      | 0.61841974  | 5.86979946  | -0.96674647 |
| Ga      | 3.23155482  | 3.05647332  | -1.04221518 |
| Ga      | 1.11175767  | 3.98997110  | 2.86001014 |
| Ga      | 3.93028275  | 0.88184102  | 1.58377508 |
| Ga      | 5.93804656  | 0.24882686  | -1.02195659 |
| Ga      | 6.29338491  | -1.88998422 | 1.58392629 |
| P       | -5.72467151 | -2.37884070 | 1.49888357 |
| P       | -5.97018974 | -0.31321079 | -1.77540363 |
| P       | -2.72707439 | -5.57739280 | 1.53649197 |
| P       | -3.28245467 | -3.15535067 | -1.73241911 |
| P       | -0.60579068 | -6.00060775 | -1.71668811 |
| P       | -4.84898642 | 3.42957831  | -1.82990736 |
| P       | -3.49043373 | 5.22281246  | 1.36876510 |
| P       | -4.30679198 | 1.29239089  | 1.37468614 |
| P       | 0.52321993  | -2.23488479 | -1.76929942 |
| P       | -0.46853924 | 2.41626846  | 1.34582007 |
| P       | -2.14789705 | 0.59403915  | -1.80054893 |
| P       | 2.06134189  | -0.55189984 | 1.47059107 |
| P       | -1.04355186 | 4.37022989  | -1.84517628 |
| P       | 1.05058117  | 4.39123700  | 1.43493156 |
| P       | 1.62672688  | 1.49473406  | -1.82832029 |
| P       | -1.51729828 | -1.44946125 | 1.48827841 |
| P       | 4.92795989  | -3.76522564 | 1.48510026 |
| P       | 3.19502098  | -5.10153965 | -1.73961467 |
| P       | 4.32753532  | -1.34762029 | -1.78077825 |
| P       | 2.74367199  | 5.24346657  | -1.87801236 |
| P       | 3.20618289  | 3.14790106  | 1.33816397 |
| P       | 0.74809589  | 6.13308232  | 1.39848042 |
| P       | 5.41755282  | 2.40832819  | -1.84979980 |
| P       | 6.22423428  | 0.41830666  | 1.41162351 |
| H       | -0.57720272 | 1.06602158  | 1.74902045 |

2-PyH\(^+\) + H\(^+\) on GaP(111):

Total DFT Energy: -8503.773885754863 Ha
| Atomic Species | Z = 1.25 | Z = 0.75 |
|----------------|----------|----------|
| H              | 4.74718571 | 6.60220694 | 0.74840067 |
| Ga             | 0.54779205 | -6.14555839 | -0.73462534 |
| P              | 0.39842211 | -6.20219164 | 1.71366134 |
| H              | -2.46531854 | -7.08466770 | -0.96653209 |
| Ga             | 4.11773161 | -4.52723375 | -0.85613175 |
| P              | -1.68184767 | -6.01050928 | -1.55479012 |
| H              | -1.68484115 | -6.12950184 | -2.99935052 |
| Ga             | 5.43964023 | -2.90039839 | -3.25552942 |
| P              | 4.39359118 | -4.44294534 | 1.57737198 |
| H              | 5.43964023 | -2.90039839 | -3.25552942 |
| Ga             | 6.78950200 | -2.88885132 | -1.29983125 |
| P              | -1.68184767 | -6.01050928 | -1.55479012 |
| H              | -4.87443433 | -3.85582360 | -3.16071156 |
| Ga             | 7.17200865 | 1.00826957 | -1.59040022 |
| P              | 5.81884026 | 0.99076981 | -3.54564536 |
| H              | -4.11742997 | 3.91202598 | -3.74246334 |
| Ga             | 2.25004520 | -0.62678439 | -3.41775206 |
| P              | -4.46747551 | 5.28492782 | -1.88416194 |
| H              | -1.10239872 | 6.90636247 | -2.01235601 |
| Ga             | -2.50517504 | 5.32914082 | 0.89578504 |
| P              | -0.54863398 | 5.52961222 | -1.86992683 |
| H              | 1.87559376 | -4.51064798 | -3.11866568 |
| Ga             | 2.63317122 | 3.25758705 | -3.69871465 |
| P              | -4.49159512 | 0.02832267 | -3.44295734 |
| H              | 7.17200865 | 1.00826957 | -1.59040022 |
| Ga             | 5.81884026 | 0.99076981 | -3.54564536 |
| P              | -4.11742997 | 3.91202598 | -3.74246334 |
| H              | -4.67647551 | 5.28492782 | -1.88416194 |
| Ga             | -1.10239872 | 6.90636247 | -2.01235601 |
| P              | -2.50517504 | 5.32914082 | 0.89578504 |
| H              | -0.54863398 | 5.52961222 | -1.86992683 |
| Ga             | 1.87559376 | -4.51064798 | -3.11866568 |
| P              | 2.63317122 | 3.25758705 | -3.69871465 |
| H              | -4.49159512 | 0.02832267 | -3.44295734 |
| Ga             | 0.54779205 | -6.14555839 | -0.73462534 |
| P              | 4.11773161 | -4.52723375 | -0.85613175 |
| Ga             | 2.71056284 | -6.02277054 | 1.84742687 |
| P              | -2.59871476 | -3.87372537 | -0.96350344 |
| Ga             | -5.77080993 | -1.64022264 | -1.05393902 |
| P              | -2.23815861 | -0.01910480 | -1.15827231 |
| Ga             | -0.26280175 | -3.95308845 | 1.72546030 |
| P              | 0.92689451 | -2.27687244 | -1.00743320 |
| Ga             | -3.68779482 | -1.50177100 | 1.55489348 |
| P              | 4.47204174 | -0.67721937 | -1.21719389 |
| Ga             | 1.34295986 | 1.59578010 | -1.44194382 |
| P              | 3.11560480 | -2.49689474 | 1.61485176 |
| Ga             | 4.87757546 | 3.17544427 | -1.42208515 |
| P              | 3.64624033 | 1.66720832 | 1.31846453 |
| Ga             | -6.66579470 | 0.60982471 | 1.32876758 |
| P              | -5.39248290 | 2.26599974 | -1.34395094 |
| Ga             | -1.83564727 | 3.82321463 | -1.52575536 |
| P              | -3.32238673 | 2.13492379 | 1.30219937 |
| Ga             | 0.41079839 | 4.04008445 | 1.54727737 |
| P              | 1.65345294 | 5.45942150 | -1.55129916 |
| Ga             | 3.80183113 | 5.29774866 | 1.02733127 |
| P              | 0.39842211 | -6.20219164 | 1.71366134 |
### Py° + H** on GaP(111):

**Total DFT Energy:** -8503.070282380731 Ha

| H[Z=1.25] | 2.34284404 | -7.26872700 | -1.20276814 |
| H[Z=1.25] | 4.51768446 | -6.87022439 | 1.75100713 |
| H[Z=1.25] | 5.61474468 | -5.09892756 | -1.33857897 |
| H[Z=1.25] | 6.96911980 | -2.66213697 | -1.56809703 |
| H[Z=1.25] | 4.96130507 | 5.25055958 | 2.06293623 |
| H[Z=1.25] | -8.32924249 | -0.57822998 | 1.24465121 |
| H[Z=1.25] | -7.21562214 | 1.24907445 | -1.84140532 |
| H[Z=1.25] | 1.44238534 | 6.99156471 | -2.20127589 |
| H[Z=1.25] | 3.62379402 | 7.28177438 | 0.76051155 |

---

**P**

| 1.87573778 | -4.39360207 | -1.66858754 |
| 5.43243601 | -2.78804362 | -1.80916948 |
| -4.86439637 | -3.74257655 | -1.71589988 |
| -6.02092766 | -1.63592249 | 1.38239547 |
| -2.64210011 | -3.68578315 | 1.44705765 |
| 2.24259281 | -0.53079582 | -1.97790294 |
| -2.08397403 | 0.16334271 | 1.27831569 |
| -1.30128125 | -2.11186164 | -1.84564228 |
| 1.35917718 | 1.90838809 | 0.92364804 |
| -4.48990065 | 0.14630712 | -1.99120398 |
| 4.49647243 | -0.53817079 | 1.20011366 |
| -0.92626602 | 1.72964164 | -2.14040453 |
| 0.86946363 | -1.93343710 | 1.42472136 |
| 5.16499711 | 3.40182567 | 0.99394798 |
| 5.81345915 | 1.09432801 | -2.09914481 |
| 2.65407311 | 3.39488598 | -2.25581451 |
| -4.09897115 | 4.01714357 | -2.29654294 |
| -1.88853692 | 4.01659872 | 0.84622270 |
| -5.59840030 | 2.66743953 | 1.06809783 |
| -0.55073120 | 5.62758544 | -2.42648923 |
| 1.58792137 | 5.93929671 | 0.81114920 |
| -0.37707627 | 2.65994669 | 5.54090869 |
| -0.41364124 | 2.71498573 | 4.03020171 |
| 1.67671078 | 3.86367542 | 4.12058774 |
| 1.94536541 | 3.33604965 | 5.35804805 |
| 0.81193279 | 2.87611182 | 6.14419190 |
| 0.91659965 | 2.78948059 | 7.22427723 |
| 2.92287964 | 3.47474160 | 5.80676611 |
| 2.43820875 | 4.43453717 | 3.58954236 |
| -1.43041932 | 2.85894985 | 3.64877296 |
| -1.27590889 | 2.40365874 | 6.09460003 |
| 0.44425113 | 3.80997931 | 3.52288998 |
| -0.05724051 | 1.74889075 | 3.61068018 |
| 0.70513927 | 0.80667203 | 1.50435255 |
| Element | Charges | X-coordinate | Y-coordinate | Z-coordinate |
|---------|---------|--------------|--------------|--------------|
| H       | Z=0.75  | -1.32644895  | -7.37142663  | -0.99178528  |
| H       | Z=0.75  | -0.71820941  | -6.29556038  | -3.02313803  |
| H       | Z=0.75  | 5.79999853   | -1.97228499  | -3.29374258  |
| H       | Z=0.75  | 7.14062547   | -1.75427516  | -1.34381782  |
| H       | Z=0.75  | -4.22984672  | -4.55804126  | -3.15946624  |
| H       | Z=0.75  | -4.84421160  | -5.63153989  | -1.12917345  |
| H       | Z=0.75  | -2.68655805  | -5.34712402  | 1.64771279   |
| H       | Z=0.75  | 2.28836527   | -0.23482594  | -3.43093268  |
| H       | Z=0.75  | -1.21036656  | 1.49622016   | -3.56804914  |
| H       | Z=0.75  | -0.96474498  | -2.39245678  | -3.2954738   |
| H       | Z=0.75  | 5.96318127   | 0.32839282   | 1.29982869   |
| H       | Z=0.75  | 6.89640442   | 2.15523353   | -1.6165465   |
| H       | Z=0.75  | 5.55346297   | 1.93081861   | -3.56605193  |
| H       | Z=0.75  | -4.72199722  | 3.23364826   | -3.70567113  |
| H       | Z=0.75  | -5.48311487  | 4.49212822   | -1.83815844  |
| H       | Z=0.75  | -2.21342211  | 6.66244587   | -1.97358173  |
| H       | Z=0.75  | -3.33243223  | 4.86969555   | 0.93263705   |
| H       | Z=0.75  | -1.45690156  | 5.39932277   | -3.84036042  |
| H       | Z=0.75  | 2.53847110   | -4.13000022  | -3.14963700  |
| H       | Z=0.75  | 2.04683358   | 3.66215387   | -3.69413965  |
| H       | Z=0.75  | -4.47163218  | -0.66132398  | -3.42395626  |
| Ga      |        | 1.48111072   | -5.97086674  | -0.76887243  |
| Ga      |        | 4.76439686   | -3.79933155  | -0.90730682  |
| Ga      |        | 3.64055280   | -5.50728928  | 1.81104987   |
| Ga      |        | -1.97545123  | -4.22148977  | -0.96685538  |
| Ga      |        | -5.45478255  | -2.53450730  | -1.03918125  |
| Ga      |        | -2.23058737  | -0.36006809  | -1.14804687  |
| Ga      |        | 0.38076255   | -3.94526065  | 1.71349280   |
| Ga      |        | 1.25819501   | -2.09799402  | -1.03979810  |
| Ga      |        | -3.39677751  | -2.08846968  | 1.56383760   |
| Ga      |        | 4.49618769   | 0.05933518   | -1.24139071  |
| Ga      |        | 1.04066344   | 1.80386928   | -1.42992648  |
| Ga      |        | 3.45673034   | -1.96311123  | 1.57951083   |
| Ga      |        | 4.28509489   | 3.93221937   | -1.44185305  |
| Ga      |        | 3.35536967   | 2.21678411   | 1.32566756   |
| Ga      |        | -6.68390574  | -0.46115842  | 1.37211186   |
| Ga      |        | -5.70717322  | 1.37631510   | -1.32096172  |
| Ga      |        | -2.45941310  | 3.49576088   | -1.50682434  |
| Ga      |        | -3.66016896  | 1.56508890   | 1.31746707   |
| Ga      |        | -0.25400704  | 4.03060002   | 1.41981716   |
| Ga      |        | 0.74187379   | 5.67736018   | -1.54528736  |
| Ga      |        | 2.90069388   | 5.83260277   | 1.03592855   |
| P       |        | 1.38341192   | -6.05939236  | 1.68633321   |
| P       |        | -0.73843554  | -6.17973247  | -1.57827067  |
| P       |        | 5.04470852   | -3.67481529  | 1.53082361   |
| P       |        | 2.52720791   | -4.02647457  | -1.69927416  |
| H       | Z=1.25 | 5.79153459 | -5.067538517 | -1.24294804 |
|---------|--------|------------|--------------|-------------|
| H       | Z=1.25 | 7.43831119 | -3.57503837  | 1.70135542  |
| H       | Z=1.25 | 7.46972292 | -1.5189062   | -1.40583298 |
| H       | Z=1.25 | -4.55913304 | -5.94838910  | -1.62899983 |
| H       | Z=1.25 | 1.55596660 | 6.99163062   | -2.22154269 |
| H       | Z=1.25 | -6.80908935 | -4.84433809  | 1.16804324  |
| H       | Z=1.25 | -6.79290447 | -2.73159949  | -1.93652672 |
| H       | Z=1.25 | -2.35534982 | 6.65897112   | -2.36718113 |
| H       | Z=1.25 | -0.64703593 | 8.06213309   | 0.58658361  |
| H       | Z=0.75 | 2.70541541  | -7.05261609  | -1.02387129 |
| H       | Z=0.75 | 2.67438333  | -5.83558517  | -3.06527320 |

Py^* + 2H^* + 2H_2O^* + 2OH^* on GaP(111):
Total DFT Energy: -8808.52313101235 Ha
| Atom | X     | Y   | Z    |
|------|-------|-----|------|
| H[Z=0.75] | 6.01512612 | 1.23539124 | -3.38977924 |
| H[Z=0.75] | 7.04460875 | 2.13252150 | -1.44455951 |
| H[Z=0.75] | -1.22900418 | -6.16675681 | -3.20995313 |
| H[Z=0.75] | -1.20525010 | -7.38603021 | -1.16850631 |
| H[Z=0.75] | 0.48677117 | -6.00147381 | 1.60045751 |
| H[Z=0.75] | 2.11162335 | 0.90281014 | -3.53444780 |
| H[Z=0.75] | -1.77755391 | 0.57189507 | -3.67918343 |
| H[Z=0.75] | 0.44362079 | -2.62541861 | -3.37176004 |
| H[Z=0.75] | 4.95130577 | 3.32811090 | 1.18317480 |
| H[Z=0.75] | 4.81289772 | 5.34844120 | -1.75108740 |
| H[Z=0.75] | 3.78501071 | 4.44479543 | -3.69626261 |
| H[Z=0.75] | -5.68094142 | 0.24072344 | -3.82386336 |
| H[Z=0.75] | -6.98858677 | 0.94016198 | -1.96627800 |
| H[Z=0.75] | -5.31332891 | 4.48766982 | -2.12814274 |
| H[Z=0.75] | -5.35143408 | 2.40010248 | 0.79630807 |
| H[Z=0.75] | -4.00831645 | 3.78206163 | -3.98567028 |
| H[Z=0.75] | 4.34105480 | -2.29795213 | -3.21902856 |
| H[Z=0.75] | -0.11152579 | 4.11029824 | -3.83194230 |
| H[Z=0.75] | -3.45227236 | -2.96068593 | -3.50843622 |
| Ga     | 4.38425895 | -4.39147954 | -0.81191704 |
| Ga     | 6.06582704 | -0.84102242 | -0.99183581 |
| Ga     | 5.96914836 | -2.86725615 | 1.75101600 |
| Ga     | 0.50547001 | -4.69612406 | -1.02084170 |
| Ga     | -3.33732496 | -5.04728805 | -1.06396210 |
| Ga     | -1.71462870 | -1.53740201 | -1.3625735 |
| Ga     | 2.38788949 | -3.21991100 | 1.64027347 |
| Ga     | 2.18092951 | -1.17723488 | -1.11639482 |
| Ga     | -1.79395415 | -3.69997208 | 1.71524948 |
| Ga     | 3.83482953 | 2.33954535 | -1.34560403 |
| Ga     | -0.02533793 | 2.03127716 | -1.50963720 |
| Ga     | 3.96854744 | 0.13058150 | 1.47932464 |
| Ga     | 1.63677357 | 5.52635667 | -1.51300166 |
| Ga     | 1.72051193 | 3.67543765 | 1.39828522 |
| Ga     | -5.47325215 | -3.88340137 | 1.30029246 |
| Ga     | -5.57444677 | -1.81051996 | -1.37677185 |
| Ga     | -3.88959006 | 1.66724069 | -1.60919502 |
| Ga     | -4.11602658 | -0.52997337 | 1.65075435 |
| Ga     | -2.32459088 | 3.30100686 | 1.31679079 |
| Ga     | -2.24859558 | 5.19354322 | -1.63811372 |
| Ga     | -0.49534972 | 6.54753639 | 1.25546040 |
| P      | 4.33339784 | -4.51101141 | 1.63401607 |
| P      | 2.58946846 | -5.73042997 | -1.62093241 |
| P      | 6.20063327 | -0.57662658 | 1.45303183 |
| P      | 4.26338045 | -2.20328481 | -1.76923416 |
| P      | 5.93405696 | 1.33666762 | -1.94577267 |
| P      | -1.30116925 | -6.06495059 | -1.76557960 |

59
| Symbol | X       | Y       | Z       |
|--------|---------|---------|---------|
| P      | -3.54716609 | -5.20679725 | 1.33600615 |
| P      | 0.40337479  | -4.56590874  | 1.36727429 |
| P      | 2.03764663  | 0.99864860   | -2.09332047 |
| P      | -2.00777108 | -1.46631543  | 1.00132252 |
| P      | 0.37666979  | -2.51659431  | -1.93179994 |
| P      | -0.16958302 | 2.34384271   | 0.85731812 |
| P      | -3.54573938 | -2.88119488  | -2.06117566 |
| P      | 3.76838756  | 2.48343404   | 1.04089346 |
| P      | -1.83642098 | 0.66863802   | -2.24183900 |
| P      | 1.90695156  | -0.95773140  | 1.31724013 |
| P      | 1.75762636  | 5.91870385   | 0.81693864 |
| P      | 3.70250724  | 4.54904887   | -2.25162060 |
| P      | -0.18077866 | 4.23885142   | -2.38295186 |
| P      | -5.73060346 | 0.34199922   | -2.37961233 |
| P      | -4.05531341 | 1.74692172   | 0.76086593 |
| P      | -6.06687669 | -1.65872866  | 0.96732885 |
| P      | -4.05216477 | 3.87889268   | -2.53171961 |
| P      | -2.58034190 | 5.53319330   | 0.68243849 |
| C      | -2.49558708 | 1.99152316   | 5.49075780 |
| C      | -2.71620855 | 2.17587786   | 4.13082512 |
| C      | -1.55999940 | 4.19184663   | 4.14201499 |
| C      | -1.29472432 | 4.07426221   | 5.50222186 |
| C      | -1.76299904 | 2.95125049   | 6.18941780 |
| H      | -1.56530206 | 2.83182720   | 7.24983009 |
| H      | -0.73319009 | 4.85453400   | 6.00322956 |
| H      | -1.22296240 | 5.05068675   | 3.57417273 |
| H      | -3.27543561 | 1.45629283   | 3.54923022 |
| H      | -2.89223768 | 1.10797616   | 5.97801447 |
| N      | -2.24721085 | 3.24802334   | 3.46714763 |
| H      | -0.00607896 | 1.08463609   | 1.46499993 |
| O      | 1.65910861  | 3.69851734   | 3.55338786 |
| H      | -0.93564507 | -0.75550175  | 1.57255328 |
| H      | 0.81269888  | 3.36519328   | 3.89650351 |
| H      | 2.34346198  | 3.12658996   | 3.94020326 |
| H      | 0.14188765  | 6.55203857   | 3.56634809 |
| O      | -4.17713704 | -0.60621869  | 3.56124138 |
| H      | -3.27854640 | -0.57360005  | 3.92143244 |
| O      | -0.51155832 | 7.09650474   | 3.10382347 |
| O      | -1.85235450 | -3.37362010  | 3.82423165 |
| H      | -2.00511242 | -4.20796474  | 4.30093424 |
| H      | -1.00124405 | -3.03901328  | 4.15492458 |

2-PyH⁺ + 2H⁺ + 2H₂O⁺ + 2OH⁻ on GaP(111):

Total DFT Energy: -8809.23508085191 Ha

H[Z=1.25] 5.78627258 -5.07644929 -1.24386920
H[Z=1.25] 7.43438908 -3.58541404 1.70045039
| H[Z=1.25] | 7.46906859 | -1.52997163 | -1.40715960 |
| H[Z=1.25] | -4.56544571 | -5.94398384 | -1.63179232 |
| H[Z=1.25] | 1.56645526 | 6.98801482 | -2.22581449 |
| H[Z=1.25] | -6.81453066 | -4.83644916 | 1.16457422 |
| H[Z=1.25] | -6.79500550 | -2.72438020 | -1.94043213 |
| H[Z=1.25] | -2.34525800 | 6.66036962 | -2.37216011 |
| H[Z=1.25] | -0.63572142 | 8.06194273 | 0.58165157 |
| H[Z=0.75] | 2.69755245 | -7.05745276 | -1.02499193 |
| H[Z=0.75] | 2.66849471 | -5.84080825 | -3.06665321 |
| H[Z=0.75] | 6.01841860 | 1.22578600 | -3.39196778 |
| H[Z=0.75] | 7.04867180 | 2.12199314 | -1.44673049 |
| H[Z=0.75] | -1.23528792 | -6.16697562 | -3.21203905 |
| H[Z=0.75] | -1.21351107 | -7.38585320 | -1.17033383 |
| H[Z=0.75] | 0.47974555 | -6.00290314 | 1.59867757 |
| H[Z=0.75] | 2.11451890 | 0.89820933 | -3.53734197 |
| H[Z=0.75] | -1.77505315 | 0.57228018 | -3.68278075 |
| H[Z=0.75] | 0.44193507 | -2.62781312 | -3.37425100 |
| H[Z=0.75] | 4.95639167 | 3.32082881 | 1.18033934 |
| H[Z=0.75] | 4.82111709 | 5.34072443 | -1.75437071 |
| H[Z=0.75] | 3.79250510 | 4.43799972 | -3.69956180 |
| H[Z=0.75] | -5.67883578 | 0.24611282 | -3.82816659 |
| H[Z=0.75] | -6.98594617 | 0.94762431 | -1.97098646 |
| H[Z=0.75] | -5.30608234 | 4.49293484 | -2.13325699 |
| H[Z=0.75] | -5.34745960 | 2.40602784 | 0.79162062 |
| H[Z=0.75] | -4.00161279 | 3.78525711 | -3.99037854 |
| H[Z=0.75] | 4.33975781 | -2.30535975 | -3.22081402 |
| H[Z=0.75] | -0.10443259 | 4.10849985 | -3.83594535 |
| H[Z=0.75] | -3.45436008 | -2.95810236 | -3.51163075 |

Ga
- 4.37996427 | -4.39760538 | -0.81313396 |
Ga
- 6.06563436 | -0.84822605 | -0.99313227 |
Ga
- 5.96560830 | -2.87445349 | 1.74935447 |
Ga
- 0.49950979 | -4.69684812 | -1.01966800 |
Ga
-3.34260117 | -5.04218053 | -1.06743467 |
Ga
-1.71281191 | -1.53171029 | -1.36439948 |
Ga
2.38501576 | -3.22764873 | 1.63972899 |
Ga
2.17991563 | -1.18163106 | -1.11635853 |
Ga
-1.80559971 | -3.68508827 | 1.71226049 |
Ga
3.83565327 | 2.33689282 | -1.33766712 |
Ga
-0.01363352 | 2.03504314 | -1.55718949 |
Ga
3.96920556 | 0.13367693 | 1.47527382 |
Ga
1.64313896 | 5.52270266 | -1.50469511 |
Ga
1.67727221 | 3.64757026 | 1.40530115 |
Ga
-5.47298787 | -3.87870413 | 1.30381114 |
Ga
-5.57458420 | -1.80238573 | -1.37122022 |
Ga
-3.88478060 | 1.67344213 | -1.60623048 |
Ga
-4.10574360 | -0.47375280 | 1.65778705 |
|     | X          | Y          | Z          |
|-----|------------|------------|------------|
| Ga  | -2.29394269| 3.28530639 | 1.41798918 |
| Ga  | -2.24200291| 5.19209308 | -1.62495254|
| Ga  | -0.49349774| 6.55216329 | 1.26868075 |
| P   | 4.33030571 | -4.51958434| 1.63258011 |
| P   | 2.58270933 | -5.73476043| -1.62174353|
| P   | 6.19956674 | -0.58400148| 1.45075793 |
| P   | 4.26180501 | -2.20956078| -1.77069850|
| P   | 5.93443983 | 1.33028380 | -1.94674794|
| P   | -1.30757335| -6.06443304| -1.76750424|
| P   | -3.54995541| -5.20611209| 1.33211451 |
| P   | 0.39414793 | -4.56534794| 1.37025924 |
| P   | 2.04676060 | 0.99241508 | -2.10065289|
| P   | -2.01367372| -1.45155776| 0.99838923 |
| P   | 0.37454371 | -2.51793228| -1.93398112|
| P   | -0.16894228| 2.32182751 | 0.77420594 |
| P   | -3.54689861| -2.87526999| -2.06329572|
| P   | 3.76058719 | 2.48672571 | 1.05054263 |
| P   | -1.83530508| 0.67149342 | -2.25091378|
| P   | 1.91046930 | -0.96504315| 1.31718987 |
| P   | 1.75708422 | 5.89685578 | 0.83015221 |
| P   | 3.70815806 | 4.54408968 | -2.25362824|
| P   | -0.17491923| 4.24692297 | -2.39422544|
| P   | -5.72743742| 0.34845109 | -2.38246866|
| P   | -4.04134454| 1.77201658 | 0.75686757 |
| P   | -6.04470618| -1.64745144| 0.98139864 |
| P   | -4.04517840| 3.88313888 | -2.53622859|
| P   | -2.56015543| 5.50574754 | 0.69446477 |
| C   | -1.33654915| 1.93396153 | 5.42709469 |
| C   | -1.44385521| 1.92292103 | 3.92016379 |
| C   | -1.59364545| 4.30380000 | 4.02254566 |
| C   | -0.92922096| 4.31929400 | 5.23243309|
| C   | -0.98033528| 3.09335333 | 6.01948182 |
| H   | -0.82040870| 3.15002760 | 7.09463906 |
| H   | -0.67994314| 5.27232274 | 5.68672787 |
| H   | -1.83727934| 5.23794884 | 3.52643520|
| H   | -2.04013708| 1.08423389 | 3.55208936 |
| H   | -1.48802589| 1.01348843 | 5.98386363 |
| N   | -2.04387810| 3.18074921 | 3.41319386 |
| H   | -0.43298245| 1.80757885 | 3.48313277 |
| H   | 0.04482671 | 1.05956846 | 1.35567855 |
| O   | 1.57315073 | 3.61917140 | 3.53885098 |
| H   | -0.93166969| -0.76287682| 1.57889898 |
| H   | 0.73005311 | 3.99129313 | 3.90927238 |
| H   | 1.57762932 | 2.70051517 | 3.86056153 |
| H   | -0.15717848| 6.47332605 | 3.64356115 |
| O   | -4.08894438| -0.47767643| 3.56893438 |
2-PyH* + 2H* + 2H2O* + 2OH* + CO2 TS on GaP(111):
Total DFT Energy: -899.7645055076912 Ha

H[Z=1.25] 5.10633912 -5.90081462 -1.09849254
H[Z=1.25] 6.88048746 -4.55779157 1.84381311
H[Z=1.25] 7.25533902 -2.61897112 -1.31589132
H[Z=1.25] -5.25771973 -5.38108522 -1.71268599
H[Z=1.25] 2.57417265 6.58656157 -2.50411559
H[Z=1.25] -7.93905795 -3.89880278 0.99800279
H[Z=1.25] -7.02563027 -1.90178170 -2.16097906
H[Z=1.25] -1.34218427 6.78314236 -2.73596934
H[Z=1.25] 0.48054284 8.02958576 0.21969649
H[Z=0.75] 1.77472126 -7.44156091 -0.90130885
H[Z=0.75] 1.95158534 -6.29329915 -2.97487075
H[Z=0.75] 6.23047852 0.24641879 -3.40807513
H[Z=0.75] 7.33255120 1.05355749 -1.46320597
H[Z=0.75] -1.95673604 -6.09629189 -3.20561351
H[Z=0.75] -2.14111432 -7.24578558 -1.13212266
H[Z=0.75] -0.33327632 -6.02109698 1.63896686
H[Z=0.75] 2.32185157 0.44204675 -3.63877142
H[Z=0.75] -1.57235897 0.63737946 -3.86923067
H[Z=0.75] 0.18573137 -2.82093128 -3.42187194
H[Z=0.75] 5.36830891 2.60017384 1.07963773
H[Z=0.75] 5.56654191 4.53175093 -1.91042715
H[Z=0.75] 4.46516104 3.71794482 -3.85503761
H[Z=0.75] -5.48067951 0.83438726 -4.09997345
H[Z=0.75] -6.71858804 1.76004213 -2.29428360
H[Z=0.75] -4.57267110 5.04115380 -2.51070271
H[Z=0.75] -4.95469379 3.06663268 0.46706846
H[Z=0.75] -3.33821293 4.10974729 -4.31623286
H[Z=0.75] 4.08748556 -3.02055974 -3.18312920
H[Z=0.75] 0.56298940 3.91099918 -4.07652970
H[Z=0.75] -3.71588897 -2.62875640 -3.64432349
C -2.38916999 2.32240721 5.16162376
C -1.88772170 2.27896456 3.76687086
C -1.51683062 4.63247598 3.90736919
C -1.59058679 4.60977591 5.28072472
C -2.15717159 3.44063135 5.89848494
H -2.45587872 3.48213058 6.94363231
H -1.37694083 5.50532905 5.85263959
H -1.28754991 5.54639842 3.36789185
H  -2.41368752  1.56822000  3.13267475
H  -2.86342775  1.43714721  5.57242929
N  -1.80977465  3.55693854  3.13022838
H  -0.79966307  1.78480533  3.77431637
O  -0.70469636 -0.44932647  4.10579444
C   0.11453776  0.41203541  4.00745446
O   1.23888587  0.82836828  4.03658449
Ga  3.79534817 -5.02843634 -0.72156100
Ga  5.95067087 -1.73754223 -0.93872469
Ga  5.52565807 -3.65096919  1.83194218
Ga -0.08633231 -4.81152315 -1.01098895
Ga -3.93859871 -4.63549564 -1.13668383
Ga -1.83705804 -1.39254729 -1.50889815
Ga  1.90822695 -3.50719829  1.65109423
Ga  2.06236785 -1.56331936 -1.17437044
Ga -2.28458489 -3.40865485  1.64978312
Ga  4.17379744  1.70201376 -1.43798755
Ga  0.31658352  1.90340758 -1.71724376
Ga  3.93635679 -0.41898494  1.43384648
Ga  2.43786374  5.14856694 -1.75001862
Ga  2.18059135  3.38028042  1.20895951
Ga -5.94351921 -3.11021859  1.15342682
Ga -5.70365417 -1.13744380 -1.59803259
Ga -3.55872805  2.06986456 -1.86503642
Ga -4.13118533  0.03572685  1.42278415
Ga -1.82460079  3.59375571  1.10913485
Ga -1.45128824  5.33864725 -1.96179927
Ga  0.38998394  6.52930570  0.94291008
P   3.67437800 -5.04730943  1.73192740
P   1.85093682 -6.13540042 -1.53615479
P   6.05814586 -1.41412700  1.49469113
P   3.99993314 -2.87327160 -1.73928983
P   6.13094913  0.40378964 -1.96606254
P  -2.04677601 -5.94185058 -1.76574070
P  -4.21917177 -4.68975924  1.27080728
P  -0.22687204 -4.59198008  1.36817540
P   2.23402763  0.58402775 -2.20489947
P  -2.1699906 -1.20690542  0.83041525
P   0.10674185 -2.66873198 -1.98964733
P   0.15858490  2.30702666  0.61292786
P  -3.82713637 -2.49371063 -2.20254117
P   4.07521421  1.92915102  0.94633880
P  -1.65243695  0.78317908 -2.44104213
P   1.74991720 -1.21964528  1.23331031
P   2.54852970  5.58173022  0.57434415
P   4.36564563  3.87717454 -2.41450046
### Py$^+$ + 4H$_2$O$^+$ on CdTe(111):

**Total DFT Energy:** $-4290.288699739292$ Ha

| Z  | x    | y    | z    |
|----|------|------|------|
| 1.5| -8.74412866 | 0.02127361 | -1.89744196 |
| 1.5| -9.42620564 | -2.38884482 | 1.73620925  |
| 1.5| -7.63096282 | -4.52364144 | -1.68470957 |
| 1.5| 4.18264146 | -7.96036032 | -1.44176659 |
| 1.5| 2.71350952 | 9.22264161 | 1.30525944  |
| 1.5| 4.64069026 | 7.21514893 | -2.12056784 |
| 1.5| 7.56564085 | -4.72242832 | -1.56127597 |
| 1.5| 6.70868793 | -7.08199726 | 2.06735974  |
| 1.5| 0.13742835 | 8.52687322 | -2.20887484 |
| 0.5| -7.47687743 | 4.20859324 | -1.81966259 |
| 0.5| -6.30704186 | 2.91199652 | -1.4569227 |
| 0.5| -4.08695287 | -6.15262706 | -3.73464233 |
| 0.5| -5.19772636 | -1.61891222 | -3.91318653 |
| 0.5| -4.57727824 | -7.63116871 | -1.26598083 |
| 0.5| -2.93261972 | 6.14202809 | -4.27608367 |
| 0.5| -4.08840645 | 7.44968272 | -1.94021694 |
| 0.5| -0.71135115 | -2.92333975 | -3.85202011 |
| 0.5| 2.66172129 | 0.30333313 | -3.97235889 |
| 0.5| 1.55192820 | 4.83723437 | -4.15190513 |
| 0.5| -1.82265915 | 1.60764867 | -4.06552545 |
| 0.5| -0.07442600 | -8.94086909 | -1.17370646 |
| 0.5| 3.77201379 | -4.22734074 | -3.72685558 |
| 0.5| 0.39860942 | -7.45771917 | -3.64146188 |
| 0.5| 6.95791973 | 1.6224328 | 1.70293670 |
| 0.5| 6.03732414 | 3.53260428 | -4.09073654 |

P: phosphorus; O: oxygen; H: hydrogen; Z: coordination number.
| Elemental | Symbol | Z | x  | y  | z   |
|-----------|--------|---|----|----|-----|
| Hydrogen  | H[Z=0.5] | 7.62909751 | 4.04309991 | -1.69886996 |
| Hydrogen  | H[Z=0.5] | -2.00593709 | -6.95441212 | 2.02042545 |
| Hydrogen  | H[Z=0.5] | 8.74054211 | -0.50831379 | -1.48703462 |
| Hydrogen  | H[Z=0.5] | 7.14708327 | -1.00081217 | -3.88119424 |
| Hydrogen  | H[Z=0.5] | -4.95590337 | 5.08925097 | 1.45739046 |
| Cadmium   | Cd | -6.99043159 | 0.49586854 | -1.26207828 |
| Cadmium   | Cd | -5.87982887 | -4.07218031 | -1.07649144 |
| Cadmium   | Cd | -4.49951625 | 1.06210686 | 1.77440770 |
| Cadmium   | Cd | -7.53051466 | -1.93958357 | 1.66859280 |
| Cadmium   | Cd | -3.48670784 | -3.13238379 | 1.66837019 |
| Cadmium   | Cd | -3.68688058 | 3.66975011 | -1.49675744 |
| Cadmium   | Cd | -0.35576995 | 6.81851160 | -1.45718798 |
| Cadmium   | Cd | 0.76421725 | 2.35908794 | -1.30447457 |
| Cadmium   | Cd | 2.19413598 | 7.35733277 | 1.66207862 |
| Cadmium   | Cd | -2.57131469 | -0.82423583 | -1.20308414 |
| Cadmium   | Cd | -0.93474967 | 4.42881348 | 1.74538539 |
| Cadmium   | Cd | -1.48458367 | -5.34326981 | -1.03744595 |
| Cadmium   | Cd | 1.85987907 | -2.10980791 | -1.13778940 |
| Cadmium   | Cd | 3.14670021 | 3.36662852 | 1.55416941 |
| Cadmium   | Cd | 2.91200384 | -6.64369470 | -0.91534299 |
| Cadmium   | Cd | 4.42102036 | -1.52289849 | 1.62196120 |
| Cadmium   | Cd | 1.30856076 | -4.55050894 | 1.75799359 |
| Cadmium   | Cd | 5.35892383 | -5.68704713 | 1.93654514 |
| Cadmium   | Cd | 4.13727299 | 5.51272002 | -1.41085428 |
| Cadmium   | Cd | 5.22817957 | 1.06998915 | -1.26542616 |
| Cadmium   | Cd | 6.32319157 | -3.37763396 | -1.02716450 |
| Tellurium | Te | -7.27922031 | 0.77809595 | 1.54791849 |
| Tellurium | Te | -6.31350166 | 2.99347455 | -2.39418057 |
| Tellurium | Te | -6.03741594 | -4.23386943 | 1.76840062 |
| Tellurium | Te | -5.20391320 | -1.53163248 | -2.11325722 |
| Tellurium | Te | -4.08714846 | -6.06674070 | -1.96364991 |
| Tellurium | Te | -2.92992683 | 6.22444543 | -2.5112943 |
| Tellurium | Te | -0.53959008 | 7.16411701 | 1.32209337 |
| Tellurium | Te | -3.72653959 | 3.78130137 | 1.30716202 |
| Tellurium | Te | -0.72911444 | -2.82375006 | -2.08379898 |
| Tellurium | Te | 0.68509387 | 2.17364942 | 1.51146012 |
| Tellurium | Te | -1.82445659 | 1.68936914 | -2.30368326 |
| Tellurium | Te | 1.67025888 | -1.82015194 | 1.69731941 |
| Tellurium | Te | 1.54060428 | 4.91046594 | -2.35858218 |
| Tellurium | Te | -1.49490648 | -5.22211168 | 1.80913679 |
| Tellurium | Te | 2.64144320 | 0.39760849 | -2.20875423 |
| Tellurium | Te | -2.30953773 | -0.65121295 | 1.61966544 |
| Tellurium | Te | 2.87488521 | -6.83629852 | 1.93798288 |
| Tellurium | Te | 0.36066612 | -7.36154061 | -1.87343039 |
| Tellurium | Te | 3.74675083 | -4.13449112 | -1.92824137 |
| Tellurium | Te | 6.02196361 | 3.60198944 | -2.32427836 |
2-PyH⁺ + 4H₂O⁺ on CdTe(111):  
Total DFT Energy: -4290.986109451165 Ha

|          | X            | Y            | Z            |
|----------|--------------|--------------|--------------|
| Te       | 5.19165240   | 1.22746829   | 1.56582894   |
| Te       | 4.45740550   | 5.78302824   | 1.37307762   |
| Te       | 7.11972294   | -0.90117337  | -2.11241495  |
| Te       | 6.59979923   | -3.25030656  | 1.81181477   |
| C        | -1.97330351  | 5.33901140   | 6.15434498   |
| C        | -1.54929987  | 5.40607223   | 4.82913654   |
| C        | -1.42652845  | 3.09668337   | 4.67529707   |
| C        | -1.84510144  | 2.94057237   | 5.99350554   |
| C        | -2.12540947  | 4.08378351   | 6.74675135   |
| H        | -2.45742601  | 3.99868299   | 7.77642251   |
| H        | -1.94888233  | 1.94502976   | 6.41047414   |
| H        | -1.41372141  | 6.35736765   | 4.32150175   |
| H        | -2.17750244  | 6.25129251   | 6.70404691   |
| N        | -1.28528634  | 4.30605066   | 4.10393099   |
| H        | -1.20100396  | 2.23769701   | 4.05008529   |
| O        | -4.22591597  | 1.34011775   | 4.22958097   |
| H        | -3.93833045  | 2.26516397   | 4.31176950   |
| H        | -3.40831393  | 0.83753312   | 4.38362613   |
| O        | 2.27126537   | 7.53995749   | 4.03661321   |
| H        | 3.19925879   | 7.69035023   | 4.27566179   |
| H        | 2.09110692   | 6.59113399   | 4.29475741   |
| O        | 3.90323417   | 3.38228997   | 4.27198395   |
| H        | 4.72268365   | 3.75948593   | 3.91165592   |
| H        | 4.01459612   | 2.42108133   | 4.18328903   |
| O        | 1.69045594   | 4.99400872   | 4.61695014   |
| H        | 1.00562292   | 4.75633625   | 3.97339684   |
| H        | 2.44834714   | 4.40432037   | 4.41397955   |

Total DFT Energy: -44290.986109451165 Ha
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|--------------|--------------|--------------|
| H[Z=0.5] | -0.71848677 | -2.92319354 | -3.85352464 |
| H[Z=0.5] | 2.66435404 | 0.29323460 | -3.97392029 |
| H[Z=0.5] | 1.56831528 | 4.83044067 | -4.15446963 |
| H[Z=0.5] | -1.81604390 | 1.61109809 | -4.06803279 |
| H[Z=0.5] | -0.10019668 | -8.94213237 | -1.17401167 |
| H[Z=0.5] | 3.76089160 | -4.24073356 | -3.72741440 |
| H[Z=0.5] | 0.37771315 | -7.46087263 | -3.64196320 |
| H[Z=0.5] | 6.96363161 | 1.60017626 | 1.70181233 |
| H[Z=0.5] | 6.04973278 | 3.51225370 | -4.09235489 |
| H[Z=0.5] | 7.4266759 | 4.01836775 | -1.70033038 |
| H[Z=0.5] | -2.02618962 | -6.94925442 | 2.01945255 |
| H[Z=0.5] | 8.74029977 | -0.53634979 | -1.48748848 |
| H[Z=0.5] | 7.14573433 | -1.02446199 | -3.88180958 |
| H[Z=0.5] | -4.93960591 | 5.10317766 | 1.45375267 |
| Cd     | -6.98690836 | 0.51912547 | -1.25675280 |
| Cd     | -5.88923659 | -4.05365535 | -1.07762995 |
| Cd     | -4.8365256 | 1.18389977 | 1.86374514 |
| Cd     | -7.53149049 | -1.90603333 | 1.67191053 |
| Cd     | -3.51976350 | -3.09930006 | 1.68079978 |
| Cd     | -3.67298980 | 3.66351474 | -1.46067387 |
| Cd     | -0.35158789 | 6.81944427 | -1.46675343 |
| Cd     | 0.77585871 | 2.37140008 | -1.30222258 |
| Cd     | 2.17226052 | 7.35652481 | 1.66876798 |
| Cd     | -2.57573486 | -0.81156473 | -1.18784686 |
| Cd     | -0.76187312 | 4.54832204 | 1.94431855 |
| Cd     | -1.49590412 | -5.34079337 | -1.03999661 |
| Cd     | 1.85080811 | -2.11387156 | -1.14412359 |
| Cd     | 3.16569008 | 3.29950149 | 1.71490659 |
| Cd     | 2.89452492 | -6.65213515 | -0.91296636 |
| Cd     | 4.40926209 | -1.55313794 | 1.62908018 |
| Cd     | 1.27291513 | -4.54643489 | 1.75538648 |
| Cd     | 5.34127268 | -5.70799813 | 1.93426794 |
| Cd     | 4.13618462 | 5.50070360 | -1.39357084 |
| Cd     | 5.22985942 | 1.06336555 | -1.26886063 |
| Cd     | 6.31436419 | -3.39623414 | -1.02737133 |
| Te     | -7.26797164 | 0.80806285 | 1.55007425 |
| Te     | -6.29967836 | 3.01181683 | -2.39561179 |
| Te     | -6.06282168 | -4.21754888 | 1.76682274 |
| Te     | -5.20753959 | -1.51554957 | -2.11510615 |
| Te     | -4.10350703 | -6.05593850 | -1.96545310 |
| Te     | -2.92340649 | 6.21976276 | -2.51646672 |
| Te     | -0.55919935 | 7.25323114 | 1.29050689 |
| Te     | -3.65896010 | 3.84490781 | 1.32921085 |
| Te     | -0.74173112 | -2.81978742 | -2.08477454 |
| Te     | 0.65985697 | 2.19175523 | 1.49268302 |
| Te     | -1.81617554 | 1.69085537 | -2.30850935 |
$\text{Te} + 1.65620688 \times -1.81679356 \times 1.69138604$

$\text{Te} + 1.54705356 \times 4.91575254 \times -2.36803302$

$\text{Te} - 1.52889879 \times -5.21060723 \times 1.80671922$

$\text{Te} + 2.64147326 \times 0.39331145 \times -2.21118933$

$\text{Te} - 2.34189994 \times -0.62302853 \times 1.63399959$

$\text{Te} + 2.84550063 \times -6.83298361 \times 1.93908931$

$\text{Te} + 0.34174295 \times -7.36469817 \times -1.87376789$

$\text{Te} + 3.73393224 \times -4.14552224 \times -1.92879113$

$\text{Te} + 6.02841670 \times 3.59379018 \times -2.32419906$

$\text{Te} + 5.20499298 \times 1.18960570 \times 1.56427185$

$\text{Te} + 4.41900511 \times 5.76260888 \times 1.38501750$

$\text{Te} + 7.11694606 \times -0.92036951 \times -2.11237252$

$\text{Te} + 6.59086599 \times -3.27651555 \times 1.81165196$

$\text{C} - 3.25703494 \times 4.93581426 \times 5.43112936$

$\text{C} - 2.24716942 \times 5.22880469 \times 4.54495016$

$\text{C} - 1.47246850 \times 2.94424464 \times 4.50771709$

$\text{C} - 2.23999610 \times 2.75402841 \times 5.80183788$

$\text{C} - 3.14602831 \times 3.69173040 \times 6.17051657$

$\text{H} - 3.74045766 \times 3.55713055 \times 7.07267731$

$\text{H} - 2.06077779 \times 1.86373792 \times 6.39883931$

$\text{H} - 2.01543403 \times 2.45168780 \times 3.67566029$

$\text{H} - 2.16031735 \times 6.23552640 \times 4.13245628$

$\text{H} - 3.96565800 \times 5.70219869 \times 5.72571473$

$\text{N} + 1.25080191 \times 4.37471428 \times 4.17207392$

$\text{H} - 0.49523342 \times 2.44816836 \times 4.55209623$

$\text{O} - 4.35445681 \times 1.03485484 \times 4.32049702$

$\text{H} + 3.92944879 \times 1.80662266 \times 4.74954041$

$\text{H} - 3.68081471 \times 0.33880090 \times 4.39675726$

$\text{O} + 2.13614097 \times 7.61126060 \times 4.01862185$

$\text{H} + 3.05765155 \times 7.60032187 \times 4.32119584$

$\text{H} + 1.75450625 \times 6.73553325 \times 4.34079844$

$\text{O} + 3.29023849 \times 3.52426438 \times 4.16292232$

$\text{H} + 4.11876469 \times 3.99635556 \times 4.34380194$

$\text{H} + 3.37939718 \times 2.66282824 \times 4.60050600$

$\text{O} + 1.21167021 \times 5.29042767 \times 4.86735299$

$\text{H} + 0.30179862 \times 4.96199051 \times 4.57415474$

$\text{H} + 1.86042378 \times 4.62226362 \times 4.56854165$

$\text{Py} + 6\text{H}_2\text{O}^*$ on CuInS$_2$(112):

Total DFT Energy: $-17453.424142286931$ Ha

$\text{H}[Z=0.25] - 3.02301659 \times 8.02141232 \times 0.86738544$

$\text{H}[Z=0.25] + 4.22980239 \times 6.20529616 \times -4.17709852$

$\text{H}[Z=0.25] + 3.54644490 \times 8.79002099 \times 1.23976797$

$\text{H}[Z=0.25] + 2.53965743 \times 6.97289289 \times -3.80570390$
| H[Z=0.25] | -0.2074498 | 0.75635135 | -3.78002116 |
| H[Z=0.25] | 3.42146693 | -0.92958911 | -3.54518490 |
| H[Z=0.25] | 0.67535542 | -7.14613933 | -3.52050719 |
| H[Z=0.25] | 1.97797799 | -8.17955526 | 1.58072609 |
| H[Z=0.25] | 7.53394557 | 5.61276514 | -1.14351750 |
| H[Z=0.25] | 6.01105719 | 7.70855373 | 1.42425335 |
| H[Z=0.25] | 6.56200744 | 1.52494800 | -3.40863854 |
| H[Z=0.25] | 3.42146693 | -0.92958911 | -3.54518490 |
| H[Z=0.25] | 0.67535542 | -7.14613933 | -3.52050719 |
| H[Z=0.25] | 1.97797799 | -8.17955526 | 1.58072609 |
| H[Z=0.25] | 7.53394557 | 5.61276514 | -1.14351750 |
| H[Z=0.25] | 6.01105719 | 7.70855373 | 1.42425335 |
| H[Z=0.25] | 6.56200744 | 1.52494800 | -3.40863854 |
| H[Z=0.75] | 5.09325082 | 7.22682646 | -2.22782105 |
| H[Z=0.75] | -3.78329701 | 2.36772341 | -3.66020074 |
| H[Z=0.75] | -2.90049261 | -5.53476727 | -3.40068677 |
| H[Z=0.75] | -0.60516695 | 4.62823124 | -3.53551444 |
| H[Z=0.75] | 1.67620559 | 7.99542311 | -1.85643844 |
| H[Z=0.75] | 2.98616449 | 3.13633208 | -3.28781821 |
| H[Z=0.75] | -3.78329701 | 2.36772341 | -3.66020074 |
| H[Z=0.75] | -2.90049261 | -5.53476727 | -3.40068677 |
| H[Z=0.75] | -0.60516695 | 4.62823124 | -3.53551444 |
| H[Z=0.75] | 1.67620559 | 7.99542311 | -1.85643844 |
| H[Z=0.75] | 2.98616449 | 3.13633208 | -3.28781821 |
| H[Z=0.75] | 3.86897230 | -4.76715852 | -3.02829224 |
| H[Z=0.75] | 0.04662847 | -8.22738713 | -1.43913851 |
| H[Z=0.75] | 6.06832682 | 3.75955170 | 1.43342577 |
| H[Z=0.75] | 6.16429288 | 5.39582797 | -3.16411982 |
| H[Z=0.75] | 6.95113463 | -4.14393890 | 1.69295173 |
| H[Z=0.75] | 7.04710577 | -2.50765061 | -2.90359394 |
| H[Z=0.75] | 7.68006903 | 1.69764582 | -1.33622118 |
| H[Z=0.75] | 6.81608488 | -7.45879048 | -1.06775589 |
| H[Z=0.75] | 8.56288193 | -6.20583275 | -1.07569530 |
| H[Z=1.5] | -6.10519928 | 7.73400819 | 0.65447266 |
| H[Z=1.5] | -6.40690911 | 0.13591842 | -2.30092444 |
| H[Z=1.5] | -6.78533609 | 3.94067087 | -2.23872451 |
| H[Z=1.5] | -8.52172787 | 6.05035647 | 0.63099032 |
| H[Z=1.5] | -8.13739686 | 2.11571266 | 0.66032933 |
| H[Z=1.5] | -5.52510469 | -7.76657560 | -2.04140535 |
| H[Z=1.5] | -5.90352318 | -3.96281106 | -1.97819351 |
| H[Z=1.5] | -7.63891498 | -1.85312211 | 0.89151620 |
| H[Z=1.5] | -7.25459246 | -5.78677802 | 0.91984330 |
| H[Z=1.5] | -2.9987565 | -9.06813399 | -1.88058995 |
| H[Z=1.5] | -1.52972034 | 8.06686888 | -2.17402525 |
| H[Z=1.5] | 0.66326565 | 8.50161359 | 1.02687231 |
| H[Z=1.5] | 3.77158924 | -8.30052190 | -1.50820055 |
| H[Z=1.5] | -0.87290886 | -8.60278727 | 1.45729119 |
| H[Z=1.5] | 5.23974456 | 8.83429563 | -1.80163072 |
| H[Z=1.5] | 5.89717064 | -7.83417860 | 1.82967372 |
| Cu | -3.17984631 | 4.64656656 | 1.02381129 |
| Cu | -5.27646660 | 4.21926728 | -1.55212884 |
| Cu | -2.68392926 | 0.6678328 | 1.03666082 |
| Cu | -6.90354221 | 6.29867567 | 0.65242214 |
| Element | X-Coordinate  | Y-Coordinate  | Z-Coordinate |
|---------|---------------|---------------|--------------|
| Cu      | -2.27231851   | -3.32852454   | 1.21140181   |
| Cu      | -4.40390730   | -3.61563196   | -1.32799822  |
| Cu      | -1.71781586   | -7.27817956   | 1.27813047   |
| Cu      | -6.03947192   | -1.76873628   | 0.89492948   |
| Cu      | 3.54420778    | 5.43004735    | 1.35348927   |
| Cu      | 1.46752679    | 5.00358033    | -1.21444185  |
| Cu      | 4.02572404    | 1.39480774    | 1.41812438   |
| Cu      | -1.59551392   | 2.58953939    | -1.38871562  |
| Cu      | -0.07037556   | 7.01898674    | 1.03160844   |
| Cu      | 4.46344835    | -2.46041664   | 1.54861369   |
| Cu      | 2.33626714    | -2.78822868   | -0.97883363  |
| Cu      | 5.01084383    | -6.52534466   | 1.62161672   |
| Cu      | -0.74205571   | -5.21998871   | -1.02132372  |
| Cu      | 0.73724050    | -0.94447686   | 1.31479377   |
| Cu      | 4.93699226    | 3.38631490    | -0.94568263  |
| Cu      | 5.86120194    | -4.42629446   | -0.70781942  |
| In      | -6.3890625    | 2.30173064    | 0.88304874   |
| In      | -5.53221412   | -5.58066544   | 0.97046876   |
| In      | -4.73616573   | 0.29283974    | -1.72831554  |
| In      | -3.86966702   | -7.58093632   | -1.46560991  |
| In      | -2.16788291   | 6.48792477    | -1.56891287  |
| In      | 0.36050094    | 3.05387413    | 1.48246828   |
| In      | -1.28752631   | -1.30955634   | -1.36973001  |
| In      | 1.33301220    | -4.83337974   | 1.58050991   |
| In      | 1.89981677    | 0.99969305    | -1.36770428  |
| In      | 2.7752477    | -6.83484319   | -1.11661905  |
| In      | 4.58710474    | 7.25896326    | -1.17805622  |
| In      | 5.51709717    | -0.48721567   | -0.98535587  |
| S       | -5.48237260   | 4.48961157    | 0.81364602   |
| S       | -5.00554184   | 0.31411943    | 0.74170438   |
| S       | -3.82217638   | 2.45744875    | -2.27722323  |
| S       | -4.35364164   | 6.12226727    | -2.63728906  |
| S       | -4.54717857   | -3.44408528   | 1.10847313   |
| S       | -4.03962628   | -7.55400113   | 0.99071069   |
| S       | -2.92477514   | -5.42352617   | -2.00947096  |
| S       | -3.52170461   | -1.70200004   | -2.38073233  |
| S       | -0.37317374   | 0.77643876    | -2.25282054  |
| S       | 1.29520319    | 5.20888373    | 1.09894305   |
| S       | -0.68371307   | 4.63971358    | -2.15297859  |
| S       | 1.76622853    | 1.07042690    | 1.07651392   |
| S       | 2.82281366    | 3.18989314    | -1.91537079  |
| S       | 2.42863996    | 6.90913822    | -2.28499239  |
| S       | -2.33283073   | 6.76872440    | 0.81897041   |
| S       | -1.95478223   | 2.76847760    | 0.90555494   |
| S       | 0.50277959    | -7.03366087   | -1.98962738  |
| S       | 2.21544595    | -2.65770608   | 1.37616801   |
2-PyH$^+$ + 6H$_2$O$^+$ on CuInS$_2$(112):
Total DFT Energy: -17454.123877259830 Ha
| H[Z=0.25] | -3.22325805 | 8.02107726 | 0.86514659 |
| H[Z=0.25] | -4.23016646 | 6.20477652 | -4.17924644 |
| H[Z=0.25] | -3.34727216 | -1.69869625 | -3.91947172 |
| H[Z=0.25] | -4.79054873 | -8.94749962 | 1.20671832 |
| H[Z=0.25] | 3.54620614  | 8.78976669  | 1.23731354  |
| H[Z=0.25] | 2.53929603  | 6.97245397  | -3.80806737 |
| H[Z=0.25] | -0.20774733 | 0.75588577  | -3.78209288 |
| H[Z=0.25] | 3.42119204  | -0.93001018 | -3.54729962 |
| H[Z=0.25] | 0.67514355  | -7.14658707 | -3.52233020 |
| H[Z=0.25] | 1.97791889  | -8.17981348 | 1.57890246  |
| H[Z=0.25] | 7.53367213  | 5.61246837  | -1.14597335 |
| H[Z=0.25] | 6.01083442  | 7.70833052  | 1.42176752  |
| H[Z=0.25] | 6.56171174  | 1.52456314  | -3.41092585 |
| H[Z=0.25] | 8.41456647  | -2.29101111 | -0.88618833 |
| H[Z=0.25] | 6.89372872  | -0.19514224 | 1.68154223  |
| H[Z=0.25] | 7.44361117  | -6.37890093 | -3.15041606 |
| H[Z=0.75] | -5.09357072 | 7.22636559  | -2.2298020  |
| H[Z=0.75] | -3.78360817 | 2.36722613  | -3.6622837 |
| H[Z=0.75] | -2.90071729 | -5.53524672 | -3.40245699 |
| H[Z=0.75] | -0.60549730 | 4.62777013  | -3.53770900 |
| H[Z=0.75] | 1.67588835  | 7.99504296  | -1.85881317 |
| H[Z=0.75] | 2.98585601  | 3.13591555  | -3.29006142 |
| H[Z=0.75] | 0.27739700  | -3.2750264  | -3.2793428 |
| H[Z=0.75] | 3.86875031  | -4.76755722 | -3.0302867 |
| H[Z=0.75] | 0.04648555  | -8.22776918 | -1.44090656 |
| H[Z=0.75] | 6.06814390  | 3.75932938  | 1.43107494  |
| H[Z=0.75] | 6.16396519  | 5.39544758  | -3.16652993 |
| H[Z=0.75] | 6.95103820  | -4.14414338 | 1.69084966  |
| H[Z=0.75] | 7.04686461  | -2.50801314 | -2.90575530 |
| H[Z=0.75] | 7.67982946  | 1.69734386  | -1.33854567 |
| H[Z=0.75] | 6.81594462  | -7.45909181 | -1.06973952 |
| H[Z=0.75] | 8.56272888  | -6.20611685 | -1.07777104 |
| H[Z=1.5]  | -6.10544379 | 7.73363688  | 0.65232421  |
| H[Z=1.5]  | -6.40715994 | 0.13544186  | -2.30280162 |
| H[Z=1.5]  | -6.78562334 | 3.94019266  | -2.24072275 |
| H[Z=1.5]  | -8.52195616 | 6.04996012  | 0.62896759  |
| H[Z=1.5]  | -8.13758487 | 2.11532118  | 0.65843198  |
| H[Z=1.5]  | -5.52526904 | -7.76703435 | -2.0430337 |
| H[Z=1.5]  | -5.90372391 | -3.96327141 | -1.97994296 |
| H[Z=1.5]  | -7.63905675 | -1.85350059 | 0.88974222 |
| H[Z=1.5]  | -7.25469399 | -5.78715166 | 0.91819466  |
| H[Z=1.5]  | -2.99902247 | -9.06856184 | -1.88224390 |
| H[Z=1.5]  | -1.53004716 | 8.06626360  | -2.17631294 |
| H[Z=1.5]  | 0.66302383  | 8.50132302  | 1.02450835  |
| H[Z=1.5]  | 3.77144512  | -8.30086899 | -1.51007007 |
| H[Z=1.5]  | -0.87234916 | -8.60307833 | 1.45556178  |
| Element | Coordinates | Distance | Angle |
|---------|-------------|----------|-------|
| H[Z=1.5] | 5.23942044 8.83395310 -1.80413396 |
| H[Z=1.5] | 5.89711503 -7.83433891 1.82772873 |
| Cu | -3.14830792 4.62722278 0.99912968 |
| Cu | -5.26399219 4.20710406 -1.57276304 |
| Cu | -2.69259541 0.65234821 1.05400841 |
| Cu | -6.90100521 6.29254704 0.64707659 |
| Cu | -2.26993169 -3.33731421 1.19406158 |
| Cu | -4.40429040 -3.61364473 -1.32896313 |
| Cu | -1.71817065 -7.29785470 1.27259941 |
| Cu | -6.03949100 -1.77003733 0.89454955 |
| Cu | 3.53049158 5.42604217 1.35209844 |
| Cu | 1.45342178 5.00049209 -1.20793935 |
| Cu | 4.01861625 1.37623184 1.42965013 |
| Cu | -1.57409708 2.58032918 -1.35733972 |
| Cu | -0.07003591 7.02254383 -1.02031746 |
| Cu | 4.46041968 -2.45026302 1.55129114 |
| Cu | 2.33801626 -2.76376069 -0.95483851 |
| Cu | 5.01511201 -6.52076873 1.62075853 |
| Cu | -0.73517676 -5.21692827 -1.03198608 |
| Cu | 0.73058965 -0.92769411 1.33269051 |
| Cu | 4.94942398 3.36551758 -0.97870669 |
| Cu | 5.85578065 -4.42064321 -0.70972977 |
| In | -6.39671873 2.30509873 0.86243461 |
| In | -5.53205626 -5.58052711 0.96701910 |
| In | -4.73602664 0.29804446 -1.72181741 |
| In | -3.86895389 -7.57996948 -1.46825051 |
| In | -2.16756188 6.48676909 -1.57258474 |
| In | 0.33971281 3.05416474 1.59240515 |
| In | -1.28020695 -1.29958203 -1.37457208 |
| In | 1.33767991 -4.82861083 1.57327045 |
| In | 1.91031678 1.01056457 -1.32903103 |
| In | 2.77775241 -6.83243660 -1.11943692 |
| In | 4.58246899 7.25670458 -1.18470089 |
| In | 5.51538905 -0.48950433 -0.97894620 |
| S | -5.46662605 4.48936161 0.79721161 |
| S | -5.01269293 0.31400911 0.75427357 |
| S | -3.80326743 2.45571517 -2.27887602 |
| S | -4.35294238 6.12424931 -2.64260085 |
| S | -4.54603473 -3.44489943 1.10969904 |
| S | -4.04067172 -7.55410909 0.98862756 |
| S | -2.92472955 -5.42293148 -2.01141713 |
| S | -3.51937981 -1.69576845 -2.37410087 |
| S | -0.35196861 0.78030182 -2.25122118 |
| S | 1.28113917 5.19906339 1.09871740 |
| S | -0.68812548 4.63585874 -2.15485140 |
| S | 1.76989012 1.08394918 1.10247409 |
PyH⁺ on GaP(111):

Total DFT Energy: -8503.043987679019 Ha

| Atoms | Z  | X       | Y       | Z       |
|-------|----|---------|---------|---------|
| H     | Z=1.25 | -7.17375728 | -2.07441344 | -1.55076653 |
| H     | Z=1.25 | -7.13315525  | -4.08555527  | 1.54231988  |
| H     | Z=1.25 | -5.23155975  | -5.48264556  | -1.34188697 |
| H     | Z=1.25 | -1.91916546  | 6.87839605   | -2.10147018 |
| H     | Z=1.25 | 5.16358952   | -5.54917359  | -1.33939081 |
| H     | Z=1.25 | 0.05330081   | 8.26985132   | 0.77557410  |
| H     | Z=1.25 | 2.00924142   | 6.85284134   | -2.10006769 |
| H     | Z=1.25 | 7.14948834   | -2.16600663  | -1.54776550 |
| H     | Z=1.25 | 7.08130816   | -4.17615782  | 1.54571053  |
| H     | Z=0.75 | -7.03653981  | 1.59981067   | -1.55530644 |
| H     | Z=0.75 | -5.86674687  | 0.79962418   | -3.46452712 |
| H     | Z=0.75 | -1.99689498  | -5.99022527  | -3.04839923 |
| H     | Z=0.75 | -2.00834999  | -7.22023718  | -1.01518626 |
| H     | Z=0.75 | -3.88496139  | 4.17588773   | -3.67074424 |
| H     | Z=0.75 | -5.05190027  | 4.98195617   | -1.76275062 |
| H     | Z=0.75 | -5.11134522  | 2.98451680   | 1.14485329  |
| H     | Z=0.75 | -0.01510963  | -2.61401466  | -3.25547873 |
| H     | Z=0.75 | 1.95939520   | 0.74976762   | -3.46222816 |
| H     | Z=0.75 | -1.94647584  | 0.77469097   | -3.46272772 |
| H     | Z=0.75 | -0.03800932  | -6.02100686  | 1.70370174  |
| H     | Z=0.75 | 1.91816536   | -7.24791896  | -1.01322113 |
| H     | Z=0.75 | 1.92337605   | -6.01515849  | -3.04659983 |
| H     | Z=0.75 | 3.94117960   | 4.12595122   | -3.66973981 |
| H     | Z=0.75 | 5.11644446   | 4.91657563   | -1.76072408 |
| H     | Z=0.75 | 7.05928364   | 1.51053260   | -1.55154516 |
| H     | Z=0.75 | 5.15060760   | 2.91964895   | 1.14726788  |
| H     | Z=0.75 | 5.87966536   | 0.72483380   | -3.46043072 |
| H     | Z=0.75 | -3.92836166  | -2.59260264  | -3.24754623 |
| H     | Z=0.75 | 3.89808778   | -2.64297601  | -3.24478378 |
| H     | Z=0.75 | 0.02808155   | 4.14711759   | -3.66136045 |

| Atoms | X       | Y       | Z       |
|-------|---------|---------|---------|
| Ga    | -5.84786500 | -1.27955127 | -1.08229560 |
| Ga    | -3.91034514 | -4.69511841 | -0.85321228 |
| Ga    | -5.71522720 | -3.29187446 | 1.66103870 |
| Ga    | -3.84915436 | 2.03658047 | -1.32369062 |
| Ga    | -1.92960578 | 5.39882724 | -1.48821760 |
| Ga    | 0.01422267 | 2.04522043 | -1.24149148 |
| Ga    | -3.96043831 | -0.15754137 | 1.47505399 |
| Ga    | -1.96100401 | -1.33557215 | -1.05186812 |
| Ga    | -1.82961241 | 3.50162852 | 1.27615353 |
|   |   |   |   |
|---|---|---|---|
| Ga | -0.02802877 | -4.69098933 | -0.91682999 |
| Ga | 1.94733295 | -1.35679574 | -1.05347250 |
| Ga | -2.13332869 | -3.41466163 | 1.68465246 |
| Ga | 3.85140782 | -4.74560207 | -0.84881191 |
| Ga | 2.08855986 | -3.42986563 | 1.68428218 |
| Ga | 0.04243808 | 6.62144215 | 1.00972693 |
| Ga | 2.00132097 | 5.37305752 | -1.48809651 |
| Ga | 3.87836343 | 1.98740351 | -1.32165396 |
| Ga | 1.87564796 | 3.47807860 | 1.27179410 |
| Ga | 3.96068134 | -0.20675300 | 1.47681454 |
| Ga | 5.83350863 | -1.35477427 | -1.07941319 |
| Ga | 5.67530921 | -3.36174900 | 1.66398788 |
| P  | -6.12998674 | -1.02280641 | 1.35383882 |
| P  | -5.84716013 | 0.90443475 | -2.01846349 |
| P  | -3.97705936 | -4.84269489 | 1.59942656 |
| P  | -3.92764981 | -2.49977209 | -1.79755534 |
| P  | -1.98952263 | -5.88872755 | -1.60075718 |
| P  | -3.87911543 | 4.25820807 | -2.2244638 |
| P  | -2.14453162 | 5.79931396 | 0.91743905 |
| P  | -3.86622504 | 2.22358401 | 1.07587776 |
| P  | -0.01366525 | -2.50222272 | -1.80964832 |
| P  | 0.01464667 | 2.10038190 | 1.19731705 |
| P  | -1.92498598 | 0.86087968 | -2.01346873 |
| P  | 1.82975122 | -1.13926481 | 1.38757821 |
| P  | 0.02794742 | 4.24829028 | -2.21324865 |
| P  | -0.02823709 | -4.57418382 | 1.49128250 |
| P  | 1.93895426 | 0.83841810 | -2.01367199 |
| P  | -1.84640409 | -1.12900924 | 1.38918320 |
| P  | 3.91295175 | -4.88532823 | 1.60425042 |
| P  | 1.91729180 | -5.91585907 | -1.59860822 |
| P  | 3.89785445 | -2.55025296 | -1.79482670 |
| P  | 3.93532932 | 4.20764531 | -2.22350351 |
| P  | 3.89632399 | 2.17491952 | 1.07806358 |
| P  | 2.21907684 | 5.77215685 | 0.91677082 |
| P  | 5.86167968 | 0.82930545 | -2.01456256 |
| P  | 6.11933405 | -1.09856013 | 1.35613713 |
| C  | -1.19028371 | 4.25116103 | 4.45023986 |
| C  | -1.17309671 | 2.89617661 | 4.74218331 |
| C  | 1.20144681 | 2.88350588 | 4.72447534 |
| C  | 1.22793208 | 4.23838399 | 4.43227854 |
| C  | 0.02129980 | 4.92584744 | 4.27899776 |
| H  | 0.02528204 | 5.97632724 | 4.00662260 |
| H  | 2.18143243 | 4.73477435 | 4.30194762 |
| H  | 2.08496497 | 2.26907268 | 4.83627867 |
| H  | -2.06103843 | 2.29136867 | 4.87102225 |
| H  | -2.14014020 | 4.75871801 | 4.33728368 |
| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| N    | 0.01201554| 2.26678228| 4.87211599|
| H    | 0.00840666| 1.27055265| 5.08263806|

**DHP\textsubscript{(aq)} + CO\textsubscript{2}(aq) Transition State:**

Total DFT Energy: $-438.105123234625$ Ha, $875.8$ i cm$^{-1}$

| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| H    | 2.04384819| 0.87197391| -2.04279296|
| C    | 1.51344016| 0.32246233| 1.19293833|
| C    | 2.67237142| -0.34231513| 1.45761483|
| H    | 4.43785162| -1.31404634| 0.56983937|
| H    | 3.99210477| -0.34128738| -1.69626768|
| H    | 0.47534271| -0.55306307| -0.50496023|
| H    | 0.82552535| 0.62755176| 1.97255333|
| H    | 2.95587580| -0.56505911| 2.48202490|
| C    | 1.12865024| 0.51817353| -0.20470800|
| C    | 3.54717902| -0.72617190| 0.38615452|
| N    | 2.21354799| 0.55897262| -1.09605747|
| C    | 3.31191981| -0.21793959| -0.86198313|
| C    | 0.42379204| -1.92879854| -0.80891447|
| O    | 0.22867976| -2.51520539| 0.23514934|
| O    | 0.61965294| -2.04745375| -2.00103934|
| H    | 0.37080083| 1.26880336| -0.42105889|

**DHP\textsubscript{(aq)}:**

Total DFT Energy: $-249.507366925698$ Ha

| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | -1.35233758| -0.39761536| 0.10006854|
| C    | -0.93779233| 1.02330057| -0.22421973|
| C    | 1.36048004| 0.23514276| -0.01085010|
| C    | 0.98198439| -1.06423212| -0.12269827|
| C    | -0.42806787| -1.37858501| 0.07912526|
| H    | -0.71770120| -2.41178086| 0.25857561|
| H    | 1.72299913| -1.84545523| -0.24304875|
| H    | 2.40025879| 0.54704839| -0.02501743|
| H    | -1.02448919| 1.20968532| -1.31393118|
| H    | -2.40312831| -0.60190151| 0.28287263|
| H    | 0.78701194| 2.17589925| 0.09660096|
| H    | -1.58794824| 1.75018072| 0.27178757|
| N    | 0.44159142| 1.23640806| 0.23991924|

**CO\textsubscript{2}(aq):**

Total DFT Energy: $-188.614429025041$ Ha

| Atom | x         | y         | z         |
|------|-----------|-----------|-----------|
| C    | 0.00000000| 0.00000000| 0.00000000|
| O    | 0.00000000| 0.00000000| 1.16941774|
| O    | 0.00000000| 0.00000000| -1.16941774|

**HCOOH\textsubscript{(aq)}:**

Total DFT Energy: $-189.808204723803$ Ha
### HCOO$^-_{(aq)}$
**Total DFT Energy:** -189.362204615794 Ha

|        |            |            |            |          |
|--------|------------|------------|------------|----------|
| H      | 1.25903881 | 0.04476835 | 0.29120330 | 0.00000000 |
| C      | 0.19165277 | -0.09580879| 0.06376163 | 0.00000000 |
| O      | -0.31159882| -1.16741124| -0.2026553 | 0.00000000 |
| O      | -0.53919623| 1.02999215 | 0.10138727 | 0.00000000 |
| H      | 0.03714679 | 1.78102316 | 0.32410127 | 0.00000000 |

### β-Ga$_2$O$_3$(100)
**Total DFT Energy:** -246.48057641 eV

**Unit Cell (Å):**

|          |            |            |            |            |
|----------|------------|------------|------------|------------|
| H        | 0.00000000 | 0.00000000 | 0.00000000 | 0.00000000 |
| C        | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |
| O        | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |
| O        | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |

**Direct Coordinates:**

**Ga-16 O-24**

|          |            |            |            |            |
|----------|------------|------------|------------|------------|
| 0.00000000 | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |
| 0.00000000 | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |
| 0.00000000 | 0.25670000 | 0.00000000 | 0.00000000 | 0.00000000 |

FROZEN
Py* on β-Ga2O3(100):
Total DFT Energy: -318.93879654 eV
Unit Cell (Å):

| X        | Y        | Z        |
|----------|----------|----------|
| 6.099999999999999   | 0.00000000000000000000000 | 0.000000000000000000000000000000000 |
| 0.00000000000000000000000 | 5.8200000000000003 | 0.000000000000000000000000000000000 |
| 0.00000000000000000000000 | 0.000000000000000000000000000000000 | 39.8203000000000031 |

Direct Coordinates:
Ga-16 O-24 C-5 H-5 N-1

| X        | Y        | Z        |
|----------|----------|----------|
| 0.00000000000000000000000 | 0.25267000000000000000000019 | 0.352919999999999975 |
| 0.0002434757876160 | 0.0175372896406950 | 0.4292847756602175 |
| 0.2494870293886894 | 0.9987789094072564 | 0.5063656037626304 |
| 0.2500000000000000 | 0.2693700000000021 | 0.27828999999999984 |
| 0.0008924990447978 | 0.5018994482831434 | 0.5235975924131256 |
| 0.2554095268167559 | 0.5021558573255223 | 0.4501663612542582 |
| 0.7500000000000000 | 0.735579999999999988 | 0.373629999999999986 |
| 0.5000000000000000 | 0.25267000000000000000000019 | 0.352919999999999975 |
| 0.5013763889811111 | 0.0162429214704405 | 0.4293329361787859 |
| 0.7516241962162414 | 0.0029410748597546 | 0.5061955798538140 |
| 0.7500000000000000 | 0.2693700000000021 | 0.278289999999999984 |
| 0.5000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.5006427931646873 | 0.502513590580214 | 0.5286956936089275 |
| 0.7454098932406138 | 0.5028687966504383 | 0.4502711229910721 |
| 0.7500000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |
| 0.00000000000000000000000 | 0.7522900000000021 | 0.298999999999999995 |

H$_2$O* on β-Ga$_2$O$_3$(100):

Total DFT Energy: -261.34697355 eV

Unit Cell (Å):

\[
\begin{align*}
&6.0999999999999996 & 0.0000000000000000 & 0.0000000000000000 \\
&0.0000000000000000 & 5.8200000000000000 & 0.0000000000000000 \\
&0.0000000000000000 & 0.0000000000000000 & 39.8203000000000000
\end{align*}
\]

Direct Coordinates:

Ga-16 O-25 H-1

\[
\begin{align*}
&0.0000000000000000 & 0.2526700000000019 & 0.3529199999999975 \\
&-0.0023788771106557 & 0.018523229301082 & 0.4293918591249700 \\
&0.245793696851881 & 0.0085430819404786 & 0.5065562890108497 \\
&0.2500000000000000 & 0.2693700000000021 & 0.2782899999999984 \\
&0.0000000000000000 & 0.7522900000000021 & 0.2989999999999995 \\
&-0.0030956943561248 & 0.50934717521705 & 0.5835821863402714 \\
&0.799140026324052 & 0.7201450112432000 & 0.6485094886340045 \\
&0.5107694335695898 & 0.4945248942748838 & 0.5841641531624032
\end{align*}
\]
|                |                |                |                |                |                |                |                |
|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 0.5000000000000000 | 0.25267000000000019 | 0.3529199999999975 | FROZEN        |                |                |                |                |
| 0.4981166801291682 | 0.0170407810897670 | 0.429494779827694 |                |                |                |                |                |
| 0.7478313187585287 | 0.0078712237433964 | 0.5069838570869554 |                |                |                |                |                |
| 0.7500000000000000 | 0.2693700000000021 | 0.2782899999999984 | FROZEN        |                |                |                |                |
| 0.5000000000000000 | 0.7522900000000021 | 0.2989999999999995 | FROZEN        |                |                |                |                |
| 0.4940710641173969 | 0.5119501676351327 | 0.5273961155858308 |                |                |                |                |                |
| 0.7434900682735744 | 0.5038156065255266 | 0.4501446755105943 |                |                |                |                |                |
| 0.7500000000000000 | 0.7522900000000021 | 0.2989999999999995 | FROZEN        |                |                |                |                |
| 0.0000000000000000 | 0.5193200000000004 | 0.3758899999999983 | FROZEN        |                |                |                |                |
| -0.0034378873483802 | 0.5116137772807475 | 0.4761179979293448 |                |                |                |                |                |
| 0.0000000000000000 | 0.2497000000000003 | 0.2738999999999976 | FROZEN        |                |                |                |                |
| 0.2436076582731492 | 0.2867509368281693 | 0.5314748632045753 |                |                |                |                |                |
| 0.2500000000000000 | 0.7596699999999998 | 0.3243099999999970 | FROZEN        |                |                |                |                |
| 0.2491763907534447 | 0.7786591435791985 | 0.4247508711219973 |                |                |                |                |                |
| 0.0000000000000000 | 0.4856300000000005 | 0.2760299999999987 | FROZEN        |                |                |                |                |
| -0.0040550176917376 | 0.0043451840413873 | 0.4790111077293086 |                |                |                |                |                |
| 0.0000000000000000 | 0.9799799999999976 | 0.3780199999999994 | FROZEN        |                |                |                |                |
| 0.2487788433206561 | 0.2284726247806723 | 0.4265074786067479 |                |                |                |                |                |
| 0.2500000000000000 | 0.2452800000000011 | 0.3276100000000000 | FROZEN        |                |                |                |                |
| 0.2418561632847927 | 0.7300894999037172 | 0.5312880881077965 |                |                |                |                |                |
| 0.5000000000000000 | 0.5193200000000004 | 0.3758899999999983 | FROZEN        |                |                |                |                |
| 0.4970007884876728 | 0.5115900639680043 | 0.4778126857243948 |                |                |                |                |                |
| 0.5000000000000000 | 0.0249700000000005 | 0.2738999999999970 | FROZEN        |                |                |                |                |
| 0.7500945378937484 | 0.2877961503089596 | 0.5315053827134816 |                |                |                |                |                |
| 0.7500000000000000 | 0.7596699999999998 | 0.3243099999999970 | FROZEN        |                |                |                |                |
| 0.7476887414130091 | 0.7785162970154788 | 0.4247142562146632 |                |                |                |                |                |
| 0.5000000000000000 | 0.4856300000000005 | 0.2760299999999987 | FROZEN        |                |                |                |                |
| 0.4978267606607918 | 0.0044158458231612 | 0.4794205700483052 |                |                |                |                |                |
| 0.5000000000000000 | 0.9799799999999976 | 0.3780199999999994 | FROZEN        |                |                |                |                |
| 0.7467631469870368 | 0.2287972110751420 | 0.426321683733301 |                |                |                |                |                |
| 0.7500000000000000 | 0.2452800000000011 | 0.3276100000000000 | FROZEN        |                |                |                |                |
| 0.7495963942676456 | 0.7297589323444071 | 0.5322738555439593 |                |                |                |                |                |
| 0.4995268811575001 | 0.4927888622056820 | 0.5829837113930999 |                |                |                |                |                |
| 0.6534051991268520 | 0.5282744995248542 | 0.5873663238760670 |                |                |                |                |                |
| 0.4852923026680610 | 0.3269311316776694 | 0.5860523358917343 |                |                |                |                |                |