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## Supplementary Material

# A computational search of the ideal metal fragment for monohapto coordination of dihydrogen

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## BDE Matrix App

Our previous articles[1,2] outlined the procedure for obtaining hidden descriptors from bond dissociation energies (BDE) of transition metal complexes from a collection of computed DFT energies. Moreover, the original article also described the procedure to estimate hidden descriptors ($HD_k$) for new ligands and metal fragments performance of a few DFT calculations. This procedure is based on the relationship between BDEs in the initial matrix and the associated hidden descriptors. It has been now implemented in a user-friendly web application named BDE Matrix App. This is an open-access application accessible at https://maserasgroup-repo.github.io/bdeapp/.

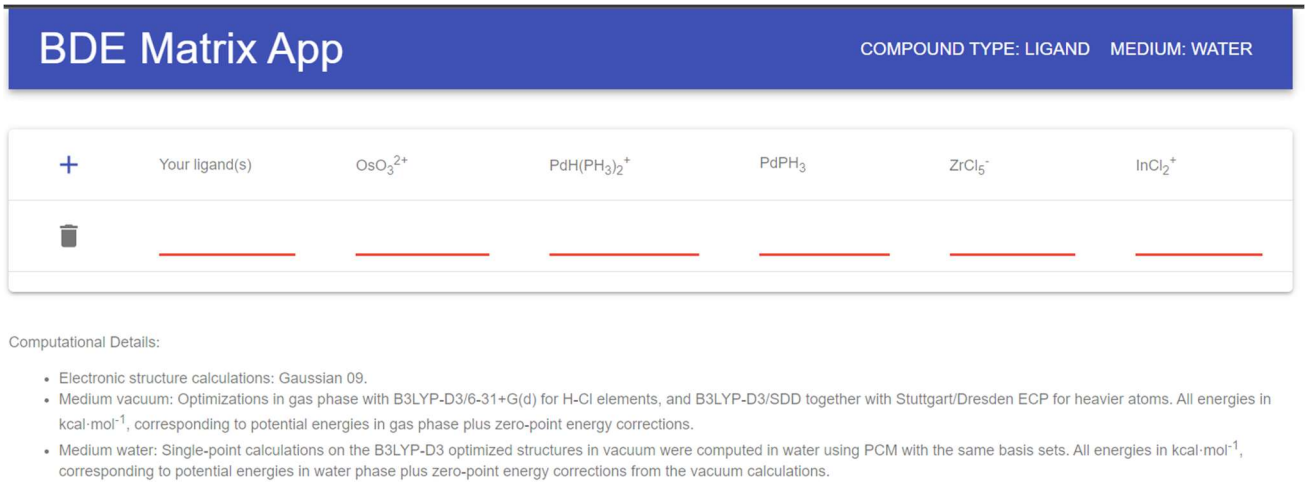


*Figure S1 BDE Matrix App.*

This application allows easy and intuitive access to the first five $HD_k$ ($k$ = 1–5) for any ligands or metal fragments whether in water or vacuum.

The concept is based on filling the gaps in the below equations in order to get hidden descriptors:

$$HDL_{k,j'} = \sum_{ref=1}^{5} \alpha_{k,ref} \cdot BDE_{ref,j'} + \beta_k \quad (1)$$

$$HDM_{k,i'} = \sum_{ref=1}^{5} \alpha_{k,ref} \cdot BDE_{i',ref} + \beta_k \quad (2)$$

Herein, $HDL_{k,j'}$ and $HDM_{i',k}$ are the values of the hidden descriptors for a new ligand ($j'$) or new metal fragment ($i'$) respectively at specific number of hidden descriptors ($k$). Therefore, HDL and HDM can be expressed as a function of the BDE of new ligand (metal fragment), $BDE_{ref,j'}$ ($BDE_{i',ref}$), with a set of metal fragments (ligands) of reference (index *ref* indicating reference moiety).

The regression parameteres $\alpha_{k,ref}$, $\beta_k$ necessary to compute the new descriptors of target chemical species, $HDL_{k,j'}$ and $HDM_{i',k}$, were obtained in the previous publications.[1,2] The set of representative reference compounds was also defined in previous publication from a set of systematic calculations.[1]

## BDE between metal fragments of reference and $\eta^1$–$H_2$, $\eta^2$–$H_2$

All the energies required to obtain the HD via the BDE Matrix App are depicted in Table S1.

*Table S1 Bond dissociation energy values in kilocalories per mole between the metal fragments of reference and $H_2$ ligand with the two coordination modes in water.*

| **Metal** | **BDE($L_nM(\eta^1–H_2)$)** | **BDE($L_nM(\eta^2–H_2)$)** |
|---|---|---|
| $OsO_3^{2+}$ | 23.56 | 20.3 |
| $PdH(PH_3)^{2+}$ | 4.20 | 1.0 |
| $PdPH_3$ | -0.57 | -6.4 |
| $ZrCl_5^-$ | 0.47 | 9.3 |
| $InCl_2^+$ | 1.48 | 0.4 |

Reported BDE($L_nM(\eta^2–H_2)$) data are from the publication Lakuntza *et al*.[1]

# Predicted BDE: Metal complex–$\eta^1$–$H_2$

*Table S2 Bond dissociation energies (kcal mol$^{-1}$) for the dihydrogen metal complex $\eta^1$–$H_2$ ligand.*

| **Metal complex** | **BDE (kcal mol$^{-1}$)** |
|---|---|
| $AuPH_3^+$ | -0.3 |
| $Co(NH_3)_5^{3+}$ | 3.4 |
| $CrO_3$ | -0.4 |
| $Cu(NH_3)_3^{2+}$ | 3.0 |
| $FeCl_2^+$ | 10.6 |
| $Fe(CO)_4$ | -2.1 |
| $IrCO(PH_3)^{2+}$ | 0.8 |
| $MnO_3^+$ | 6.1 |
| $Mo(SH)_3^+$ | 3.7 |
| $Nb(NH_2)_4^+$ | 6.7 |
| $OsO_3^{2+}$ | 21.2 |
| $PdH(PH_3)_2^+$ | 2.8 |
| $PdPH_3$ | -4.1 |
| $PtF_5^-$ | 2.9 |
| $Rh(H_2O)_5^{3+}$ | 3.7 |
| $Ru(SH_4)^+$ | 1.9 |
| $TaMe_4^+$ | 8.5 |
| $TiCl_3^+$ | 4.7 |
| $W(CO)_5$ | -2.5 |
| $ZrCl_5^-$ | 3.8 |
| $AuCl_3$ | 5.8 |
| $HgI_2$ | 15.9 |
| $InCl_2^+$ | 1.0 |

# Reported BDE: Metal complex–$\eta^2$–$H_2$

*Table S3 Bond dissociation energies (kcal mol$^{-1}$) for the dihydrogen metal complex $\eta^2$–$H_2$ ligand.*

| **Metal complex** | **BDE (kcal mol$^{-1}$)** |
|---|---|
| $AuPH_3^+$ | -4.7 |
| $Co(NH_3)_5^{3+}$ | 4.4 |
| $CrO_3$ | 3.1 |
| $Cu(NH_3)_3^{2+}$ | 1.7 |
| $FeCl_2^+$ | 11.5 |
| $Fe(CO)_4$ | -9.9 |
| $IrCO(PH_3)^{2+}$ | 3.3 |
| $MnO_3^+$ | 3.6 |
| $Mo(SH)_3^+$ | 5 |
| $Nb(NH_2)_4^+$ | 12.1 |
| $OsO_3^{2+}$ | 20.3 |
| $PdH(PH_3)_2^+$ | 1 |
| $PdPH_3$ | -6.4 |
| $PtF_5^-$ | 2.3 |
| $Rh(H_2O)_5^{3+}$ | -2.4 |
| $Ru(SH_4)^+$ | 1.8 |
| $TaMe_4^+$ | 16.2 |
| $TiCl_3^+$ | 13.8 |
| $W(CO)_5$ | -3 |
| $ZrCl_5^-$ | 9.3 |
| $AuCl_3$ | -2.2 |
| $HgI_2$ | -0.2 |
| $InCl_2^+$ | 0.4 |

Reported BDE data are from the publication Lakuntza *et al.*[1]

## Computed BDE: Metal complex–$\eta^1$–$H_2$

*Table S4 Computed bond dissociation energies (kcal mol$^{-1}$) for the dihydrogen metal complex $\eta^1$–$H_2$ ligand.*

| **Metal complexes** | **BDE$_{computed}$ ($L_nM(\eta^1–H_2)$)** |
|---|---|
| $Ir(CO)(PH_3)_2^+$ | 12.8 |
| $Co(NH_3)_5^+$ | 8.3 |
| $FeCl_2^+$ | 10.4 |
| $Mo(SH)_3^+$ | 15.9 |
| $ZrCl_5^-$ | 1.7 |
| $TiCl_3^+$ | 16.0 |
| $TaMe_4^+$ | 15.0 |
| $Nb(NH_2)_4^+$ | 5.2 |
| $CrO_3$ | 10.2 |
| $AuPH_3^+$ | 0.6 |
| $Cu(NH_3)_5^+$ | 2.5 |
| $OsO_3^{2+}$ | 23.6 |
| $PdH(PH_3)^{2+}$ | 4.3 |
| $PdPH_3$ | 0.0 |
| $InCl_2^+$ | 1.5 |

These computed energies are employed as a benchmark, and we compared them with the predicted BDE($\eta^1$–$H_2$) values. Along this data, we observed an average absolute deviation of 4.8 kcal mol$^{-1}$ and a maximum deviation of 12.2 kcal mol$^{-1}$.

# Hidden descriptors of the metal fragments

*Table S5 Hidden descriptors of the metal fragments in decreasing order.*

| **HD**$_{M1}$ = **M**$_1$ | **HD**$_{M2}$ = **M**$_2$ | **HD**$_{M3}$ = **M**$_3$ | **HD**$_{M4}$ = **M**$_4$ | **HD**$_{M5}$ = **M**$_5$ | **HD**$_{M6}$ = **M**$_6$ | **M**$_7$ |
|---|---|---|---|---|---|---|
| $HgI_2$ -0.08 | $Fe(CO)_4$ 0.31 | **$Nb(NH_2)_4^+$ 0.39** | $HgI_2$ 0.70 | $PdPH_3$ 0.39 | $Mo(SH)_3^+$ 0.40 | $IrCO(PH_3)_2^+$ 0.39 |
| $PdPH_3$ -0.10 | $PtF_5^-$ 0.28 | **$ZrCl_5^-$ 0.35** | $OsO_3^{2+}$ 0.37 | $Mo(SH)_3^+$ 0.34 | $HgI_2$ 0.35 | $OsO_3^{2+}$ 0.31 |
| **$Nb(NH_2)_4^+$ -0.11** | $AuCl_3$ 0.27 | $Ru(SH)_4$ 0.26 | **$FeCl_2^+$ 0.16** | $OsO_3^{2+}$ 0.30 | $PdPH_3$ 0.26 | **$TaMe_4^+$ 0.26** |
| **$ZrCl_5^-$ -0.11** | $W(CO)_5$ 0.22 | $HgI_2$ 0.24 | $AuCl_3$ 0.15 | $MnO_3^+$ 0.16 | $InCl_2^+$ 0.25 | $PtF_5^-$ 0.24 |
| $PdH(PH_3)_2^+$ -0.11 | $AuPH_3^+$ 0.20 | **$TaMe_4^+$ 0.23** | $PdH(PH_3)_2^+$ 0.11 | $Ru(SH)_4$ 0.16 | $Rh(H_2O)_5^{3+}$ 0.18 | $AuPH_3^+$ 0.18 |
| $W(CO)_5$ -0.12 | $PdPH_3$ 0.19 | $W(CO)_5$ 0.18 | **$Nb(NH_2)_4^+$ 0.09** | $W(CO)_5$ 0.10 | $Fe(CO)_4$ 0.16 | $PdPH_3$ 0.17 |
| $Ru(SH)_4$ -0.13 | $Rh(H_2O)_5^{3+}$ 0.17 | $IrCO(PH_3)_2^+$ 0.17 | $PtF_5^-$ 0.08 | **$ZrCl_5^-$ 0.08** | $Co(NH_3)_5^{3+}$ 0.15 | $PdH(PH_3)_2^+$ 0.15 |
| $Fe(CO)_4$ -0.14 | $PdH(PH_3)_2^+$ 0.15 | $Mo(SH)_3^+$ 0.17 | **$TaMe_4^+$ 0.05** | **$Nb(NH_2)_4^+$ 0.07** | **$FeCl_2^+$ 0.12** | $Co(NH_3)_5^{3+}$ 0.09 |
| $Cu(NH_3)_3^{2+}$ -0.15 | $Ru(SH)_4$ 0.13 | $PtF_5^-$ 0.15 | $Cu(NH_3)_3^{2+}$ 0.04 | $AuPH_3^+$ 0.06 | $AuPH_3^+$ 0.10 | $Cu(NH_3)_3^{2+}$ 0.03 |
| $IrCO(PH_3)_2^+$ -0.15 | $IrCO(PH_3)_2^+$ 0.12 | $Fe(CO)_4$ 0.15 | $Ru(SH)_4$ 0.03 | $Fe(CO)_4$ 0.05 | $IrCO(PH_3)_2^+$ 0.08 | $W(CO)_5$ 0.02 |
| **$TaMe_4^+$ -0.16** | $HgI_2$ 0.06 | $PdH(PH_3)_2^+$ 0.14 | $Co(NH_3)_5^{3+}$ 0.01 | $IrCO(PH_3)_2^+$ 0.03 | $TiCl_3^+$ 0.08 | $Rh(H_2O)_5^{3+}$ 0.02 |
| $AuPH_3^+$ -0.18 | $Co(NH_3)_5^{3+}$ 0.05 | $PdPH_3$ 0.12 | $IrCO(PH_3)_2^+$ -0.04 | $AuCl_3$ 0.00 | $W(CO)_5$ 0.05 | **$FeCl_2^+$ 0.02** |
| **$FeCl_2^+$ -0.20** | $Cu(NH_3)_3^{2+}$ 0.04 | $CrO_3$ 0.09 | $Rh(H_2O)_5^{3+}$ -0.05 | $HgI_2$ -0.01 | $PdH(PH_3)_2^+$ 0.01 | $Mo(SH)_3^+$ -0.02 |
| $Co(NH_3)_5^{3+}$ -0.20 | $MnO_3^+$ 0.02 | $Co(NH_3)_5^{3+}$ 0.07 | **$ZrCl_5^-$ -0.06** | $PdH(PH_3)_2^+$ -0.02 | $Cu(NH_3)_3^{2+}$ -0.01 | $Ru(SH)_4$ -0.02 |
| $Mo(SH)_3^+$ -0.21 | $InCl_2^+$ 0.01 | $Cu(NH_3)_3^{2+}$ 0.06 | $Fe(CO)_4$ -0.07 | **$TiCl_3^+$ -0.05** | **$TaMe_4^+$ -0.01** | **$ZrCl_5^-$ -0.02** |
| $PtF_5^-$ -0.21 | $CrO_3$ -0.01 | $TiCl_3^+$ 0.01 | $AuPH_3^+$ -0.10 | $Rh(H_2O)_5^{3+}$ -0.06 | $OsO_3^{2+}$ -0.12 | $InCl_2^+$ -0.06 |
| $CrO_3$ -0.22 | $OsO_3^{2+}$ - 0.19 | $AuPH_3^+$ 0.01 | $MnO_3^+$ -0.11 | **$FeCl_2^+$ -0.07** | $AuCl_3$ -0.14 | $AuCl_3$ -0.10 |
| $TiCl_3^+$ -0.24 | **$FeCl_2^+$ -0.23** | **$FeCl_2^+$ 0.00** | $W(CO)_5$ -0.11 | $PtF_5^-$ -0.08 | $Ru(SH)_4$ -0.14 | $TiCl_3^+$ -0.10 |
| $AuCl_3$ -0.25 | $Mo(SH)_3^+$ -0.24 | $AuCl_3$ -0.01 | $Mo(SH)_3^+$ -0.19 | $CrO_3$ -0.09 | **$Nb(NH_2)_4^+$ -0.18** | **$Nb(NH_2)_4^+$ -0.11** |
| $InCl_2^+$ -0.27 | **$Nb(NH_2)_4^+$ -0.25** | $Rh(H_2O)_5^{3+}$ -0.13 | $PdPH_3$ -0.21 | $TaMe_4^+$ -0.19 | $MnO_3^+$ -0.24 | $Fe(CO)_4$ -0.23 |
| $Rh(H_2O)_5^{3+}$ -0.29 | **$ZrCl_5^-$ -0.26** | $InCl_2^+$ -0.18 | $InCl_2^+$ -0.22 | $Cu(NH_3)_3^{2+}$ -0.34 | **$ZrCl_5^-$ -0.25** | $CrO_3$ -0.25 |
| $MnO_3^+$ -0.35 | $TiCl_3^+$ -0.36 | $MnO_3^+$ -0.25 | $TiCl_3^+$ -0.23 | $InCl_2^+$ -0.39 | $CrO_3$ -0.25 | $HgI_2$ -0.35 |
| $OsO_3^{2+}$ -0.42 | **$TaMe_4^+$ -0.37** | $OsO_3^{2+}$ -0.50 | $CrO_3$ -0.25 | $Co(NH_3)_5^{3+}$ -0.47 | $PtF_5^-$ -0.45 | $MnO_3^+$ -0.50 |

Reported data **M**$_1$–**M**$_7$ data are from the publication Lakuntza *et al.*[1]

## Search of the ideal metal fragment for $L_nM(\eta^1–H_2)$

The equations (1) and (2) predict the BDE for the bond between hypothetical metal fragments and the $\eta^1–H_2$($\eta^2–H_2$) ligand:

$$BDE(L_nM-(\eta^1-H_2))_{pred} = -22.935\,HDM_1 - 11.832\,HDM_2 - 1.870\,HDM_3 + 21.528\,HDM_4 + 1.504\,HDM_5 \quad (1)$$

$$BDE(L_nM-(\eta^2-H_2))_{pred} = -19.877\,HDM_1 - 32.436\,HDM_2 + 5.270\,HDM_3 + 19.458\,HDM_4 - 1.645\,HDM_5 \quad (2)$$

To fill the missing values of $HD_{Mk}$, we selected all possible $HD_{Mk}$ values between -0.65 to 0.65 with a step of 0.05. For $HDM_1$, and given the previous observation the range was constratined to values between -0.65 to -0.05 We computed the predicted BDEs for all the 6908733 combinations, each consisting of five numbers that refer to $HD_{M1}$, $HD_{M2}$, $HD_{M3}$, $HD_{M4}$ and $HD_{M5}$.

The procedure to identify the $L_nM$ for the formation of stable metal complexes with the end-on-bonded ligand is explained in the main text. Figure S2 depicts a 3-D representation of the Figure 4 in the main text. The big markers with the diamond shape represent our set of twenty-three metal fragments and the small dots correspond to the values for the hypothetical ideal metal fragments to form $L_nM(\eta^1–H_2)$ complexes. Regarding this 3-D representation none of the selected 23 metal fragments fall into the grid area of the 'ideal' metal fragment for the formation of the $L_nM(\eta^1–H_2)$.

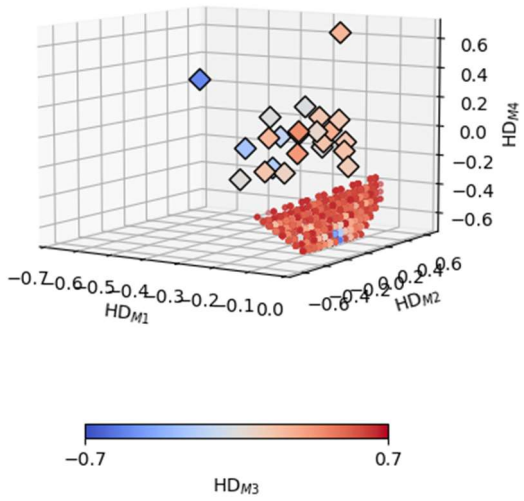


*Figure S2 3-D plot of the hidden descriptor for metal complexes $HD_{Mk}$. The diamond-shaped big dots correspond to the 23 metal fragments explicitly considered in this study, and the remaining points correspond to predicted values for the potentially stable $L_nM(\eta^1–H_2)$.*

## Cartesian coordinates and potential energies

h2_eta1_pdhph32_aq
Energy (POTENTIAL) = -511970.13992467197 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0219 | 2.8726 | 0.0331 |
| 2 | H | -0.0152 | 2.1244 | 0.0367 |
| 3 | Pd | -0.0001 | 0.0755 | -0.0106 |
| 4 | P | 2.3327 | -0.1829 | 0.0092 |
| 5 | P | -2.3329 | -0.1821 | 0.0091 |
| 6 | H | -0.0004 | -1.4467 | 0.0463 |
| 7 | H | 3.1150 | 0.9883 | 0.0009 |
| 8 | H | 2.8756 | -0.8667 | 1.1113 |
| 9 | H | 2.8978 | -0.8974 | -1.0623 |
| 10 | H | -3.1155 | 0.9888 | -0.0006 |
| 11 | H | -2.8976 | -0.8981 | -1.0616 |
| 12 | H | -2.8756 | -0.8648 | 1.1119 |

h2_eta1_pdph3_aq
Energy (POTENTIAL) = -296354.22764477396 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | -4.1061 | -0.0324 | -0.0002 |
| 2 | H | -3.3688 | 0.0742 | 0.0003 |
| 3 | Pd | -0.5351 | -0.0018 | -0.0000 |
| 4 | P | 1.6618 | 0.0021 | 0.0001 |
| 5 | H | 2.3891 | -0.8344 | -0.8866 |
| 6 | H | 2.3853 | 1.1901 | -0.2827 |
| 7 | H | 2.3893 | -0.3453 | 1.1683 |

h2_eta1_zrcl5_aqEnergy (POTENTIAL) = -1.47450533171097E6 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.3151 | 0.0645 | -4.0475 |
| 2 | H | 0.3179 | 0.0704 | -3.3037 |
| 3 | Zr | -0.0044 | -0.0016 | 0.0539 |
| 4 | Cl | -0.0900 | -0.0217 | 2.4362 |
| 5 | Cl | 0.0179 | -2.3298 | -0.7179 |
| 6 | Cl | 0.0260 | 2.3399 | -0.6783 |
| 7 | Cl | -2.4217 | 0.0085 | -0.4483 |
| 8 | Cl | 2.4409 | -0.0013 | -0.2861 |

h2_eta1_incl2_aq
Energy (POTENTIAL) = -579340.6859813051 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0000 | 2.3967 | 0.0000 |
| 2 | H | -0.0000 | 3.1466 | 0.0000 |
| 3 | In | 0.0000 | -0.0062 | 0.0000 |
| 4 | Cl | -2.2105 | -0.1540 | 0.0000 |
| 5 | Cl | 2.2105 | -0.1540 | 0.0000 |

h2_aq

Energy (POTENTIAL) = -737.6810188275683 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | -1.5058 | 1.7117 | 0.0000 |
| 2 | H | -2.2486 | 1.7117 | 0.0000 |

h2_eta1_oso3_aq
Energy (POTENTIAL) = -198890.29500194397 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0007 | 0.0067 | 1.9911 |
| 2 | H | -0.0006 | 0.0125 | 2.8242 |
| 3 | Os | 0.0000 | 0.0000 | 0.0972 |
| 4 | O | -1.2500 | -0.9578 | -0.5065 |
| 5 | O | -0.2042 | 1.5596 | -0.5115 |
| 6 | O | 1.4540 | -0.6044 | -0.5072 |

h2_eta1_oso3_vacuum

Energy (POTENTIAL) = -198614.93390510927 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.9153 | -0.3450 | -0.0015 |
| 2 | H | 1.7418 | -0.4500 | 0.0016 |
| 3 | Os | -0.9634 | -0.1054 | -0.0012 |
| 4 | O | -1.7650 | -1.5893 | 0.0002 |
| 5 | O | -1.4619 | 0.7523 | 1.3628 |
| 6 | O | -1.4650 | 0.7532 | -1.3635 |

h2_eta1_pdhph32_vacuum
Energy (POTENTIAL) = -511919.2570081243 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0225 | 2.8660 | 0.0547 |
| 2 | H | -0.0146 | 2.1178 | 0.0583 |
| 3 | Pd | 0.0004 | 0.0689 | 0.0109 |
| 4 | P | 2.3332 | -0.1895 | 0.0307 |
| 5 | P | -2.3325 | -0.1886 | 0.0307 |
| 6 | H | 0.0000 | -1.4533 | 0.0679 |
| 7 | H | 3.1155 | 0.9816 | 0.0225 |
| 8 | H | 2.8760 | -0.8733 | 1.1328 |
| 9 | H | 2.8982 | -0.9041 | -1.0407 |
| 10 | H | -3.1150 | 0.9823 | 0.0209 |
| 11 | H | -2.8972 | -0.9046 | -1.0400 |
| 12 | H | -2.8752 | -0.8713 | 1.1335 |

h2_eta1_pdph3_vacuum

Energy (POTENTIAL) = -296349.34265261673 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | -4.1064 | -0.0324 | -0.0002 |
| 2 | H | -3.3691 | 0.0742 | 0.0004 |
| 3 | Pd | -0.5355 | -0.0018 | 0.0000 |
| 4 | P | 1.6615 | 0.0021 | 0.0001 |
| 5 | H | 2.3888 | -0.8341 | -0.8868 |
| 6 | H | 2.3850 | 1.1901 | -0.2823 |
| 7 | H | 2.3890 | -0.3456 | 1.1682 |

h2_eta1_zrcl5_vacuum

Energy (POTENTIAL) = -1.4744535223455608E6 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.3150 | 0.0645 | -4.0456 |
| 2 | H | 0.3178 | 0.0704 | -3.3019 |
| 3 | Zr | -0.0045 | -0.0016 | 0.0558 |
| 4 | Cl | -0.0900 | -0.0217 | 2.4381 |
| 5 | Cl | 0.0178 | -2.3298 | -0.7160 |
| 6 | Cl | 0.0260 | 2.3399 | -0.6764 |
| 7 | Cl | -2.4218 | 0.0085 | -0.4465 |
| 8 | Cl | 2.4409 | -0.0013 | -0.2843 |

h2_vac

Energy (POTENTIAL) = -737.6269681533167 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | -1.5058 | 1.7117 | 0.0000 |
| 2 | H | -2.2486 | 1.7117 | 0.0000 |

h2_eta1_incl2_vacuum

Energy (POTENTIAL) = -579340.6859813051 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0000 | 2.3967 | 0.0000 |
| 2 | H | -0.0000 | 3.1466 | 0.0000 |
| 3 | In | 0.0000 | -0.0062 | 0.0000 |
| 4 | Cl | -2.2105 | -0.1540 | 0.0000 |
| 5 | Cl | 2.2105 | -0.1540 | 0.0000 |

zrcl5-H2eta1_aq

Energy (POTENTIAL) = -1.4745040588257604E6 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Zr | 0.0005 | 0.0175 | -0.2292 |
| 2 | Cl | -0.0271 | -0.1334 | 2.1824 |
| 3 | Cl | 0.0076 | 2.4412 | -0.2860 |
| 4 | Cl | -0.0039 | -2.3979 | -0.4373 |
| 5 | Cl | 2.4791 | 0.0120 | -0.2269 |
| 6 | Cl | -2.4785 | 0.0256 | -0.2819 |
| 7 | H | 0.1062 | 0.1536 | -3.4110 |
| 8 | H | 0.1499 | 0.1677 | -4.1520 |

ircoph32_H2eta1_aq
Energy (POTENTIAL) = -567963.2867853874 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ir | -0.0000 | -0.2273 | 0.0012 |
| 2 | C | -0.0002 | 1.6487 | -0.0033 |
| 3 | P | -2.3598 | -0.2633 | 0.0013 |
| 4 | P | 2.3599 | -0.2630 | 0.0013 |
| 5 | O | -0.0002 | 2.7951 | -0.0058 |
| 6 | H | -3.0256 | 0.9746 | -0.0166 |
| 7 | H | -2.9775 | -0.9241 | -1.0787 |
| 8 | H | -2.9785 | -0.8932 | 1.0990 |
| 9 | H | 3.0254 | 0.9750 | 0.0213 |
| 10 | H | 2.9779 | -0.9256 | 1.0799 |
| 11 | H | 2.9785 | -0.8908 | -1.0977 |
| 12 | H | -0.0021 | -2.2050 | -0.0072 |
| 13 | H | -0.0028 | -2.9551 | 0.0027 |

fecl2-H2eta1_aq
Energy (POTENTIAL) = -655995.3702150888 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Fe | -0.0174 | 0.0046 | -0.0299 |
| 2 | Cl | 0.4571 | 1.0625 | 1.7909 |
| 3 | Cl | -0.4475 | 1.0013 | -1.8957 |
| 4 | H | -0.0253 | -2.0193 | -0.0217 |
| 5 | H | -0.0141 | -2.7732 | 0.0036 |

ticl3_H2eta1_aq
Energy (POTENTIAL) = -903668.9791694487 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ti | 0.0007 | -0.0014 | 0.2950 |
| 2 | Cl | 1.9024 | -0.7617 | -0.2320 |
| 3 | Cl | -0.2890 | 2.0245 | -0.2349 |
| 4 | Cl | -1.6119 | -1.2619 | -0.2353 |
| 5 | H | -0.0275 | 0.0083 | 2.3475 |
| 6 | H | -0.0120 | 0.0070 | 3.0986 |

cro3-H2eta1_aq
Energy (POTENTIAL) = -196941.5288390144 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Cr | -0.9695 | 0.0223 | 0.0000 |
| 2 | O | -1.2684 | -1.5321 | 0.0000 |
| 3 | O | -1.3443 | 0.7814 | 1.3317 |
| 4 | O | -1.3441 | 0.7815 | -1.3316 |
| 5 | H | 0.9405 | 0.0766 | -0.0004 |
| 6 | H | 1.6838 | 0.1107 | 0.0005 |

nbnh24-H2eta1_aq
Energy (POTENTIAL) = -176939.68243025217 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Nb | -0.0000 | -0.0152 | -0.0263 |
| 2 | N | 0.0009 | 1.9307 | -0.0938 |
| 3 | N | -0.0003 | -0.3764 | 1.8956 |
| 4 | N | -1.7404 | -0.5063 | -0.8178 |
| 5 | N | 1.7399 | -0.5080 | -0.8177 |
| 6 | H | 0.0017 | 2.5652 | 0.7039 |
| 7 | H | 0.0017 | 2.4616 | -0.9678 |
| 8 | H | -0.8363 | -0.5540 | 2.4542 |
| 9 | H | 0.8356 | -0.5548 | 2.4542 |
| 10 | H | -2.4641 | 0.1935 | -0.9866 |
| 11 | H | -2.0471 | -1.4021 | -1.1937 |
| 12 | H | 2.0458 | -1.4041 | -1.1936 |
| 13 | H | 2.4643 | 0.1911 | -0.9865 |
| 14 | H | -0.0046 | -2.9713 | -0.4183 |
| 15 | H | -0.0047 | -3.7113 | -0.4903 |

mosh3_H2eta1_aq
Energy (POTENTIAL) = -794197.5437810427 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Mo | -1.4550 | 0.0045 | -0.0000 |
| 2 | S | -1.4519 | -2.2466 | -0.0000 |
| 3 | S | -2.3832 | 0.5112 | 2.0086 |
| 4 | S | -2.3828 | 0.5112 | -2.0088 |
| 5 | H | -2.7811 | -2.5525 | -0.0004 |
| 6 | H | -2.7437 | 1.7815 | 1.6692 |
| 7 | H | -2.7449 | 1.7809 | -1.6689 |
| 8 | H | 0.5760 | -0.0319 | 0.0003 |
| 9 | H | 1.3261 | -0.0584 | 0.0004 |

conh35-H2eta1_aq
Energy (POTENTIAL) = -269495.2082348608 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Co | 0.0009 | 0.0001 | -0.1757 |
| 2 | N | -2.0336 | 0.0692 | -0.2254 |
| 3 | N | 0.0449 | -0.1465 | 1.7945 |
| 4 | N | 2.0307 | -0.0023 | -0.3131 |
| 5 | N | 0.0386 | 2.0220 | -0.1017 |
| 6 | N | -0.0438 | -2.0169 | -0.3231 |
| 7 | H | -2.4741 | -0.7646 | -0.6383 |
| 8 | H | -2.4856 | 0.1782 | 0.6923 |
| 9 | H | -2.4043 | 0.8499 | -0.7858 |
| 10 | H | 0.8506 | -0.6796 | 2.1493 |
| 11 | H | 0.0862 | 0.7597 | 2.2813 |
| 12 | H | -0.7745 | -0.6269 | 2.1905 |
| 13 | H | 2.4000 | 0.7433 | -0.9206 |
| 14 | H | 2.5222 | 0.1308 | 0.5806 |
| 15 | H | 2.4295 | -0.8653 | -0.7078 |
| 16 | H | 0.0180 | 2.4642 | -1.0324 |
| 17 | H | -0.7547 | 2.4414 | 0.4014 |
| 18 | H | 0.8733 | 2.4165 | 0.3522 |
| 19 | H | -0.0827 | -2.3533 | -1.2965 |
| 20 | H | 0.7724 | -2.4930 | 0.0834 |
| 21 | H | -0.8504 | -2.4592 | 0.1371 |
| 22 | H | -0.0334 | 0.0986 | -2.0732 |
| 23 | H | -0.0603 | 0.1363 | -2.8322 |

cunh33-H2eta1_aq
Energy (POTENTIAL) = -230906.20988753877 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Cu | 0.0231 | 0.1974 | 2.3234 |
| 2 | N | 2.0091 | 0.1649 | 2.0969 |
| 3 | N | -1.9157 | 0.6262 | 2.0922 |
| 4 | N | -0.0660 | -0.5403 | 4.2282 |
| 5 | H | 2.5343 | 0.4437 | 2.9341 |
| 6 | H | 2.3248 | 0.8028 | 1.3538 |
| 7 | H | 2.3707 | -0.7606 | 1.8317 |
| 8 | H | -2.3642 | 1.0186 | 2.9285 |
| 9 | H | -2.4813 | -0.1901 | 1.8249 |
| 10 | H | -2.0730 | 1.3205 | 1.3492 |
| 11 | H | 0.0195 | 0.1999 | 4.9360 |
| 12 | H | 0.6790 | -1.2180 | 4.4272 |
| 13 | H | -0.9479 | -1.0277 | 4.4247 |
| 14 | H | 0.0061 | 0.0310 | 0.1642 |
| 15 | H | 0.0017 | -0.0138 | -0.5860 |

pdph3-H2eta1_aq
Energy (POTENTIAL) = -296354.13263976 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Pd | 0.5775 | 0.0015 | 0.0005 |
| 2 | P | -1.6730 | -0.0011 | 0.0006 |
| 3 | H | -2.3905 | 1.0840 | -0.5600 |
| 4 | H | -2.3744 | -1.0295 | -0.6751 |
| 5 | H | -2.4033 | -0.0728 | 1.2122 |
| 6 | H | 2.4715 | -0.0212 | -0.0062 |
| 7 | H | 3.2255 | -0.0129 | -0.0034 |

auph3-H2eta1_aq
Energy (POTENTIAL) = -301177.39826104086 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Au | -0.8589 | -0.0067 | -0.0005 |
| 2 | P | -3.1618 | -0.0182 | 0.0010 |
| 3 | H | -3.7307 | -1.3012 | -0.0224 |
| 4 | H | -3.7454 | 0.5971 | 1.1194 |
| 5 | H | -3.7437 | 0.6363 | -1.0958 |
| 6 | H | 1.0594 | -0.0014 | -0.0051 |
| 7 | H | 1.8178 | 0.0126 | -0.0126 |

oso3_H2eta1_aq
Energy (POTENTIAL) = -198890.291927145 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0007 | 0.0067 | 1.9911 |
| 2 | H | -0.0006 | 0.0125 | 2.8242 |
| 3 | Os | 0.0000 | 0.0000 | 0.0972 |
| 4 | O | -1.2496 | -0.9583 | -0.5065 |
| 5 | O | -0.2049 | 1.5595 | -0.5115 |
| 6 | O | 1.4543 | -0.6037 | -0.5072 |

pdhph32-H2eta1_aq
Energy (POTENTIAL) = -511970.05753260903 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Pd | -0.0001 | 0.0760 | 0.0034 |
| 2 | P | -2.3329 | -0.1826 | -0.0042 |
| 3 | P | 2.3328 | -0.1827 | -0.0041 |
| 4 | H | 0.0000 | -1.4472 | 0.0183 |
| 5 | H | -3.1149 | 0.9878 | -0.0511 |
| 6 | H | -2.8759 | -0.9175 | -1.0728 |
| 7 | H | -2.8981 | -0.8457 | 1.0998 |
| 8 | H | 3.1155 | 0.9872 | -0.0497 |
| 9 | H | 2.8974 | -0.8475 | 1.0991 |
| 10 | H | 2.8753 | -0.9167 | -1.0736 |
| 11 | H | 0.0065 | 2.1167 | 0.0093 |
| 12 | H | -0.0018 | 2.8654 | -0.0123 |

incl2_H2eta1_aq
Energy (POTENTIAL) = -579406.640628816 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | -0.0000 | -2.3967 | 0.0000 |
| 2 | H | 0.0000 | -3.1466 | 0.0000 |
| 3 | In | 0.0000 | 0.0062 | 0.0000 |
| 4 | Cl | 2.2105 | 0.1540 | 0.0000 |
| 5 | Cl | -2.2105 | 0.1540 | 0.0000 |

tame4_H2eta1_aq
Energy (POTENTIAL) = -136592.00814942617 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ta | 0.0114 | -0.0106 | -0.5880 |
| 2 | C | -1.9483 | 0.0391 | 0.3203 |
| 3 | C | 0.0663 | 1.9490 | 0.3194 |
| 4 | C | 1.9647 | -0.0628 | 0.3342 |
| 5 | C | -0.0495 | -1.9725 | 0.3140 |
| 6 | H | -2.4446 | 0.9709 | 0.0112 |
| 7 | H | -1.9781 | -0.0243 | 1.4135 |
| 8 | H | -2.5160 | -0.8100 | -0.0911 |
| 9 | H | 0.9978 | 2.4509 | 0.0210 |
| 10 | H | -0.0158 | 1.9864 | 1.4109 |
| 11 | H | -0.7823 | 2.5051 | -0.1114 |
| 12 | H | 1.9868 | -0.0021 | 1.4278 |
| 13 | H | 2.5352 | 0.7875 | -0.0710 |
| 14 | H | 2.4633 | -0.9938 | 0.0264 |
| 15 | H | -0.9793 | -2.4739 | 0.0095 |
| 16 | H | 0.0269 | -2.0125 | 1.4059 |
| 17 | H | 0.8015 | -2.5273 | -0.1137 |
| 18 | H | 0.0505 | -0.0463 | -2.8618 |
| 19 | H | 0.0472 | -0.0374 | -3.6132 |

tame4_H2eta1_vac
Energy (POTENTIAL) = -136506.98023380872 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ta | 0.0114 | -0.0106 | -0.5880 |
| 2 | C | -1.9483 | 0.0391 | 0.3203 |
| 3 | C | 0.0663 | 1.9490 | 0.3194 |
| 4 | C | 1.9647 | -0.0628 | 0.3342 |
| 5 | C | -0.0495 | -1.9725 | 0.3140 |
| 6 | H | -2.4446 | 0.9709 | 0.0112 |
| 7 | H | -1.9781 | -0.0243 | 1.4135 |
| 8 | H | -2.5160 | -0.8100 | -0.0911 |
| 9 | H | 0.9978 | 2.4509 | 0.0210 |
| 10 | H | -0.0158 | 1.9864 | 1.4109 |
| 11 | H | -0.7823 | 2.5051 | -0.1114 |
| 12 | H | 1.9868 | -0.0021 | 1.4278 |
| 13 | H | 2.5352 | 0.7875 | -0.0710 |
| 14 | H | 2.4633 | -0.9938 | 0.0264 |
| 15 | H | -0.9793 | -2.4739 | 0.0095 |
| 16 | H | 0.0269 | -2.0125 | 1.4059 |
| 17 | H | 0.8015 | -2.5273 | -0.1137 |
| 18 | H | 0.0505 | -0.0463 | -2.8618 |
| 19 | H | 0.0472 | -0.0374 | -3.6132 |

zrcl5-H2eta1_vacuum1

Energy (POTENTIAL) = -1.474440462356437E6 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Zr | 0.0005 | 0.0175 | -0.2292 |
| 2 | Cl | -0.0271 | -0.1334 | 2.1824 |
| 3 | Cl | 0.0076 | 2.4412 | -0.2860 |
| 4 | Cl | -0.0039 | -2.3979 | -0.4373 |
| 5 | Cl | 2.4791 | 0.0120 | -0.2269 |
| 6 | Cl | -2.4785 | 0.0256 | -0.2819 |
| 7 | H | 0.1062 | 0.1536 | -3.4110 |
| 8 | H | 0.1499 | 0.1677 | -4.1520 |

ticl3_H2eta1_vacuum1

Energy (POTENTIAL) = -903597.6182490659 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ti | 0.0007 | -0.0014 | 0.2950 |
| 2 | Cl | 1.9024 | -0.7616 | -0.2320 |
| 3 | Cl | -0.2890 | 2.0245 | -0.2349 |
| 4 | Cl | -1.6119 | -1.2619 | -0.2353 |
| 5 | H | -0.0275 | 0.0083 | 2.3475 |
| 6 | H | -0.0120 | 0.0070 | 3.0986 |

nbnh24-H2eta1_vacuum
Energy (POTENTIAL) = -176884.91928553913 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Nb | 0.0079 | -0.0000 | -0.0207 |
| 2 | N | 1.9287 | 0.0066 | -0.3390 |
| 3 | N | -0.1019 | -0.0003 | 1.9317 |
| 4 | N | -0.5883 | 1.7380 | -0.7420 |
| 5 | N | -0.5761 | -1.7423 | -0.7418 |
| 6 | H | 2.6610 | 0.0088 | 0.3701 |
| 7 | H | 2.3423 | 0.0075 | -1.2743 |
| 8 | H | -0.2092 | 0.8353 | 2.5087 |
| 9 | H | -0.2034 | -0.8366 | 2.5088 |
| 10 | H | 0.0810 | 2.4644 | -0.9997 |
| 11 | H | -1.5264 | 2.0410 | -0.9990 |
| 12 | H | -1.5121 | -2.0519 | -0.9988 |
| 13 | H | 0.0982 | -2.4640 | -0.9996 |
| 14 | H | -2.9741 | -0.0073 | -0.0275 |
| 15 | H | -3.7171 | -0.0101 | -0.0032 |

mosh3_H2eta1_vacuum

Energy (POTENTIAL) = -794126.1516985134 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Mo | 0.0000 | -0.0973 | 0.3488 |
| 2 | S | -0.0002 | 2.0475 | -0.3345 |
| 3 | S | 2.0088 | -0.8626 | -0.3806 |
| 4 | S | -2.0086 | -0.8630 | -0.3805 |
| 5 | H | -0.0005 | 1.9337 | -1.6937 |
| 6 | H | 1.6696 | -2.1824 | -0.3368 |
| 7 | H | -1.6686 | -2.1826 | -0.3383 |
| 8 | H | 0.0001 | 0.5565 | 2.2720 |
| 9 | H | 0.0001 | 0.8104 | 2.9783 |

ircoph32_H2eta1_vacuum1
Energy (POTENTIAL) = -567910.1654779187 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Ir | 0.0000 | -0.2274 | 0.0003 |
| 2 | C | 0.0002 | 1.6487 | -0.0007 |
| 3 | P | -2.3598 | -0.2630 | 0.0002 |
| 4 | P | 2.3599 | -0.2635 | 0.0002 |
| 5 | O | 0.0003 | 2.7950 | -0.0010 |
| 6 | H | -3.0253 | 0.9751 | -0.0153 |
| 7 | H | -2.9776 | -0.9216 | -1.0810 |
| 8 | H | -2.9786 | -0.8948 | 1.0968 |
| 9 | H | 3.0256 | 0.9744 | 0.0226 |
| 10 | H | 2.9778 | -0.9282 | 1.0776 |
| 11 | H | 2.9784 | -0.8893 | -1.1000 |
| 12 | H | -0.0024 | -2.2051 | -0.0119 |
| 13 | H | -0.0033 | -2.9552 | -0.0035 |

fecl2-H2eta1_vacuum

Energy (POTENTIAL) = -655894.9569245775 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Fe | -0.0001 | 0.4862 | 0.0066 |
| 2 | Cl | -1.8995 | -0.5394 | -0.0036 |
| 3 | Cl | 1.8970 | -0.5438 | -0.0036 |
| 4 | H | 0.0288 | 2.5098 | -0.0165 |
| 5 | H | 0.0146 | 3.2638 | -0.0335 |

incl2_H2eta1_vacuum
Energy (POTENTIAL) = -579340.6859813051 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.0000 | 2.3967 | 0.0000 |
| 2 | H | -0.0000 | 3.1466 | 0.0000 |
| 3 | In | 0.0000 | -0.0062 | 0.0000 |
| 4 | Cl | -2.2105 | -0.1540 | 0.0000 |
| 5 | Cl | 2.2105 | -0.1540 | 0.0000 |

oso32_H2eta1_vacuum
Energy (POTENTIAL) = -198614.93390510927 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | H | 0.9153 | -0.3450 | -0.0015 |
| 2 | H | 1.7418 | -0.4500 | 0.0016 |
| 3 | Os | -0.9634 | -0.1054 | -0.0012 |
| 4 | O | -1.7650 | -1.5893 | 0.0002 |
| 5 | O | -1.4619 | 0.7523 | 1.3628 |
| 6 | O | -1.4650 | 0.7532 | -1.3635 |

cro3-H2eta1_vacuum

Energy (POTENTIAL) = -196929.92313820095 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Cr | 0.0004 | -0.0000 | 0.0765 |
| 2 | O | -1.5432 | -0.0080 | -0.2740 |
| 3 | O | 0.7647 | 1.3356 | -0.2726 |
| 4 | O | 0.7785 | -1.3276 | -0.2727 |
| 5 | H | -0.0090 | -0.0006 | 1.9873 |
| 6 | H | 0.0002 | 0.0004 | 2.7313 |

conh35-H2eta1_vacuum1
Energy (POTENTIAL) = -269088.05561031617 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Co | 0.0003 | 0.0015 | -0.1715 |
| 2 | N | -2.0006 | 0.3687 | -0.2604 |
| 3 | N | -0.0042 | -0.0829 | 1.8028 |
| 4 | N | 2.0089 | -0.3054 | -0.2718 |
| 5 | N | 0.3363 | 1.9970 | -0.1609 |
| 6 | N | -0.3410 | -1.9906 | -0.2557 |
| 7 | H | -2.5544 | -0.4045 | -0.6547 |
| 8 | H | -2.4437 | 0.5744 | 0.6449 |
| 9 | H | -2.2440 | 1.1761 | -0.8519 |
| 10 | H | 0.7087 | -0.7168 | 2.1889 |
| 11 | H | 0.1645 | 0.8232 | 2.2614 |
| 12 | H | -0.8910 | -0.4232 | 2.1988 |
| 13 | H | 2.4928 | 0.3563 | -0.8957 |
| 14 | H | 2.5028 | -0.2161 | 0.6261 |
| 15 | H | 2.2806 | -1.2308 | -0.6316 |
| 16 | H | 0.3939 | 2.4055 | -1.1054 |
| 17 | H | -0.3926 | 2.5459 | 0.3141 |
| 18 | H | 1.2141 | 2.2790 | 0.2955 |
| 19 | H | -0.4163 | -2.3505 | -1.2186 |
| 20 | H | 0.3901 | -2.5679 | 0.1804 |
| 21 | H | -1.2103 | -2.2930 | 0.2034 |
| 22 | H | 0.0062 | 0.0393 | -2.0715 |
| 23 | H | -0.0046 | 0.0548 | -2.8316 |

pdhph32-H2eta1_vacuum1
Energy (POTENTIAL) = -511919.27412032196 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Pd | -0.0001 | 0.0760 | 0.0034 |
| 2 | P | -2.3329 | -0.1826 | -0.0042 |
| 3 | P | 2.3328 | -0.1827 | -0.0041 |
| 4 | H | 0.0000 | -1.4472 | 0.0183 |
| 5 | H | -3.1149 | 0.9878 | -0.0511 |
| 6 | H | -2.8759 | -0.9175 | -1.0728 |
| 7 | H | -2.8981 | -0.8457 | 1.0998 |
| 8 | H | 3.1155 | 0.9872 | -0.0497 |
| 9 | H | 2.8974 | -0.8475 | 1.0991 |
| 10 | H | 2.8753 | -0.9167 | -1.0736 |
| 11 | H | 0.0065 | 2.1167 | 0.0093 |
| 12 | H | -0.0018 | 2.8654 | -0.0123 |

auph3-H2eta1_vacuum

Energy (POTENTIAL) = -301117.35909319663 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Au | -0.3898 | -0.0003 | 0.0001 |
| 2 | P | 1.9131 | 0.0005 | -0.0004 |
| 3 | H | 2.4886 | 0.2842 | 1.2480 |
| 4 | H | 2.4947 | -1.2196 | -0.3787 |
| 5 | H | 2.4906 | 0.9414 | -0.8673 |
| 6 | H | -2.3081 | 0.0032 | 0.0040 |
| 7 | H | -3.0665 | 0.0078 | -0.0073 |

cunh33-H2eta1_vacuum
Energy (POTENTIAL) = -230706.2346524707 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Cu | 0.0000 | -0.1783 | -0.0151 |
| 2 | N | 1.9759 | -0.4544 | -0.1412 |
| 3 | N | -1.9758 | -0.4547 | -0.1412 |
| 4 | N | -0.0002 | 1.8593 | 0.1544 |
| 5 | H | 2.4660 | 0.2512 | -0.7038 |
| 6 | H | 2.2142 | -1.3580 | -0.5720 |
| 7 | H | 2.4428 | -0.4592 | 0.7751 |
| 8 | H | -2.4662 | 0.2514 | -0.7030 |
| 9 | H | -2.4426 | -0.4605 | 0.7751 |
| 10 | H | -2.2140 | -1.3578 | -0.5730 |
| 11 | H | -0.0009 | 2.3255 | -0.7615 |
| 12 | H | 0.8190 | 2.2162 | 0.6597 |
| 13 | H | -0.8190 | 2.2158 | 0.6608 |
| 14 | H | 0.0001 | -2.2003 | 0.7604 |
| 15 | H | 0.0001 | -2.9066 | 1.0172 |

pdph3-H2eta1_vacuum
Energy (POTENTIAL) = -296352.1846234439 kcal $mol^{-1}$

| | Atom | X | Y | Z |
|---|---|---|---|---|
| 1 | Pd | 0.5775 | 0.0015 | 0.0005 |
| 2 | P | -1.6730 | -0.0011 | 0.0006 |
| 3 | H | -2.3905 | 1.0840 | -0.5600 |
| 4 | H | -2.3744 | -1.0295 | -0.6751 |
| 5 | H | -2.4033 | -0.0728 | 1.2122 |
| 6 | H | 2.4715 | -0.0212 | -0.0062 |
| 7 | H | 3.2255 | -0.0129 | -0.0034 |

## References

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