

Supplementary Material for

Computational Investigation of Adsorptive Removal of Pb²⁺ from Water by the UiO-66 Metal-Organic Framework: Comparison of Adsorption Sites on Defects and Functionalised Linkers

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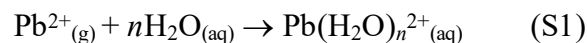
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1) Computational approach for calculating solvation free energies

To further validate our computational approach, we calculated and analyzed solvation free energies for Pb²⁺. Solvation free energies are defined as the free energy change that occurs when a solute is taken from the gas phase into the solvent^[1,2]; in the context of this study, the solvation free energy is the free energy change associated with the following reaction:



This approach for calculating the solvation free energy is well-established in the literature.^[2,3] The Gibbs free energy change of the reaction is calculated using the thermodynamic cycle thoroughly discussed in the Computational Details of the main text. To summarise this cycle, the energy of the reactants is subtracted from the energy of the products, where the free energy of the species in aqueous solution (*i.e.*, $\text{H}_2\text{O}_{(\text{aq})}$ and $\text{Pb}(\text{H}_2\text{O})_n^{2+}_{(\text{aq})}$) is calculated using the following equation:

$$G_{\text{solv}} = E_{\text{gas}}^{\text{B2}} + (G_{\text{gas}}^{\text{B1}} - E_{\text{gas}}^{\text{B1}}) + (E_{\text{solv}}^{\text{B2}} - E_{\text{gas}}^{\text{B2}}) + \Delta G^{0 \rightarrow *} \quad (\text{S2})$$

Where G_{solv} is the final solvated Gibbs free energy; E is the electronic energy; G is the Gibbs free energy; B1 indicates whether the calculation was conducted with the basis set used for optimizations and frequency calculations (for this sub-study, either aug-cc-pVDZ on H and O, aug-cc-pVDZ-PP with the Stuttgart-Koeln small-core multiconfiguration-Dirac-Hartree-Fock-adjusted (SK MCDHF RSC) ECP on Pb^[4-7] or def2-SVP on H and O. def2-TZVPP with the def2-ECP on Pb^[7-9]) and B2 indicates the basis set used for single point refinements (either aug-cc-pVDZ on H and O, aug-cc-pVDZ-PP with the SK MCDHF RSC ECP on Pb or ma-def2-TZVP on H and O, ma-def2-TZVPP with the def2- ECP on Pb); the gas and solv subscripts designate whether the calculation was conducted in gas phase or with implicit solvation, and $\Delta G^{0 \rightarrow *}$ is the concentration correction applied as described by Keith *et al.*^[10] The free energy of $\text{Pb}^{2+}_{(\text{g})}$ was calculated as follows, as solvation corrections are not required for species in gas phase:

$$G_{\text{Pb}^{2+}} = E_{\text{gas}}^{\text{B2}} + (G_{\text{gas}}^{\text{B1}} - E_{\text{gas}}^{\text{B1}}) \quad (\text{S3})$$

2) Effect of coordination number on Pb^{2+} solvation free energies

As thoroughly examined in the main text, a key aspect of modelling solvated Pb^{2+} is determining the most suitable coordination number and we found that a coordination number

of six leads to the best agreement with experiments in terms of geometry (discussion of Fig. 2 in the main text and section 3 of the Supplementary Material). Here we further examine this aspect by calculating the solvation free energy for Pb^{2+} across coordination numbers ranging from six to nine (Table S1). In addition to our analysis of the coordination number, we also tested modifying the size of the water cluster used to model the solvating water molecules in solution on the reactant side in Eqn. S1. We tested modelling these water molecules using two approaches. The first involves Pb^{2+} interacting with n non-interacting water molecules (*i.e.*, n H_2O , or the monomer approach). The second method involves modelling each water molecule as an ‘average’ water molecule taken from a larger cluster of m interacting water molecules (*i.e.*, n/m $m\text{H}_2\text{O}$, also known as the cluster model approach). We tested clusters made of $m = 6$ water molecules (*i.e.*, a hexamer cluster) and $m = 9$ (*i.e.*, a nonamer cluster). While the effect of coordination number on solvation free energies is minimal (*e.g.*, <1 kcal/mol difference in solvation free energy for coordination numbers six to eight when modelling solvating waters with hexamer and nonamer clusters), $\text{Pb}(\text{H}_2\text{O})_6^{2+}$ leads to the most accurate solvation free energy thus providing further justification for choosing this coordination number and geometry to model solvated Pb^{2+} .

There is a significant difference in solvation free energies on the order of approximately 20 kcal/mol when transitioning from a monomer approach to a water cluster model (-337.3 kcal for $\text{Pb}(\text{H}_2\text{O})_7^{2+}$ calculated using the monomer *vs.* 357.3 kcal/mol for hexamer). While this trend may appear to suggest that the monomer is the best description of liquid water, this is a spurious result driven by our chosen model chemistry which may be overestimating solvation free energies relative to the experimental value (see section 5 of the Supplementary Material). Modelling water as a monomer provides less thermodynamic driving force for solvation of Pb^{2+} to occur, hence leading to less negative solvation free energies. Therefore, we chose to use the nonamer cluster to accurately describe bulk water, in agreement with previous literature

that indicates that the water cluster approach should be used for solvation free energy calculations for charged solutes.^[11] The difference between hexamer and nonamer water clusters is much smaller (approximately 5 kcal/mol), indicating that either could potentially be used for calculating Pb^{2+} solvation energies.

Table S1. A comparison of solvation free energies with different water cluster sizes across coordination numbers 6-9. The sequential water addition energy is also presented, calculated as the energy produced by the $\text{Pb}(\text{H}_2\text{O})_{n-1}^{2+} + \text{H}_2\text{O} \rightarrow \text{Pb}(\text{H}_2\text{O})_n^{2+}$ reaction. All energies are calculated using the $\omega\text{B97X-D3BJ/def2-SVP/ma-def2-TZVP}$ ($\text{def2-TZVPP/ma-def2-TZVPP}$ on Zr, Pb) model chemistry.

Coordination number	Solvation free energy (monomer)	Solvation free energy (hexamer)	Solvation free energy (nonamer)	Sequential water addition energy (kcal/mol)
6	-339.0	-356.1	-353.2	-2.2
7	-337.3	-357.3	-353.8	-1.5
8	-334.6	-357.4	-353.5	2.6
9	-334.9	-360.6	-356.2	-3.6

3) Geometries of $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ ($n=6-9$)

We report the geometries of $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ ($n=6-9$) in order to demonstrate the transition between hemidirectionality to holodirectionality as the coordination number increases (Fig. S1). We focus on these four coordination geometries because, as demonstrated in the main text (Fig. 2), they are all thermodynamically accessible at room temperature. $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ with $n=6,7$ is hemidirected while $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ $n=8,9$ is holodirected. All geometries are optimized using the $\omega\text{B97X-D3BJ/def2-SVP}$ (def2-TZVPP with def2-ECP on Pb) model chemistry.^[7-9,12,13] As discussed in the main text, the average Pb-O bond length increases with coordination number: 2.55 Å for $\text{Pb}(\text{H}_2\text{O})_6^{2+}$, 2.62 Å for $\text{Pb}(\text{H}_2\text{O})_7^{2+}$ with, 2.66 Å for $\text{Pb}(\text{H}_2\text{O})_8^{2+}$, and 2.70 Å for $\text{Pb}(\text{H}_2\text{O})_9^{2+}$. The average bond length obtained with $\text{Pb}(\text{H}_2\text{O})_6^{2+}$ is the most consistent with the experimental value of 2.54 Å.^[14]

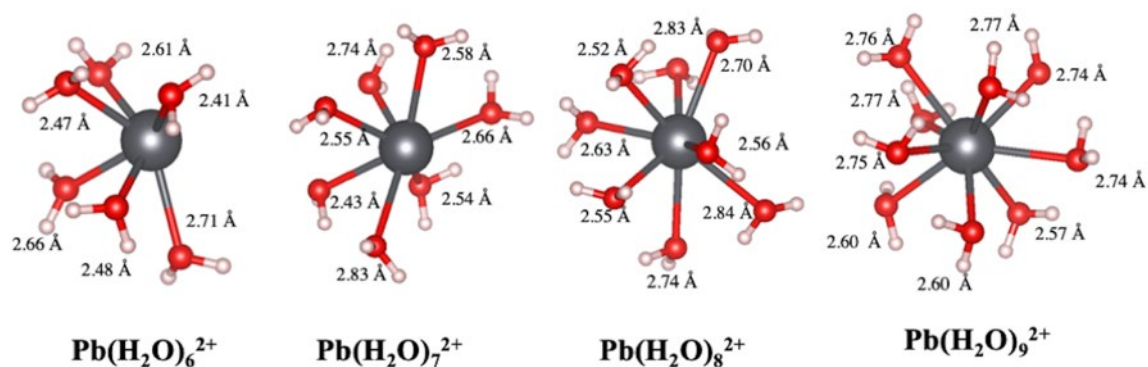


Figure S1. Visual depictions of the $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ ($n=6$ to 9) geometries along with all Pb-O bond lengths in Angstroms for each species. $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ ($n=6$ to 7) is hemidirected; $\text{Pb}(\text{H}_2\text{O})_n^{2+}$ ($n=8$ to 9) is holodirected. Pb atoms in grey, O in red, H in off-white.

4) Energetics of adsorption for fully desolvated Pb^{2+}

As discussed in the Results and Discussion section of the main text, it is plausible that Pb^{2+} could desolvate passing through the UiO-66 triangular apertures. This would have a significant effect on ΔG s and hence also on the adsorption capacity of functionalised UiO-66. This prompted us to calculate the ΔG s for the bare Pb^{2+} ion adsorbing onto functionalised linkers with no explicit solvation (Fig. S2) as an extreme case for the desolvation possibly induced by the small apertures in the UiO-66 structure. This analysis also allowed us to further validate our computational method in terms of testing whether it correctly captures the chemistry of Pb^{2+} interaction with different Lewis bases, without the confounding factors of ligand exchange thermodynamics (Fig. 4 in the main text) and the presence of water molecules affecting the electrophilicity of Pb^{2+} (Fig. 5 in the main text).

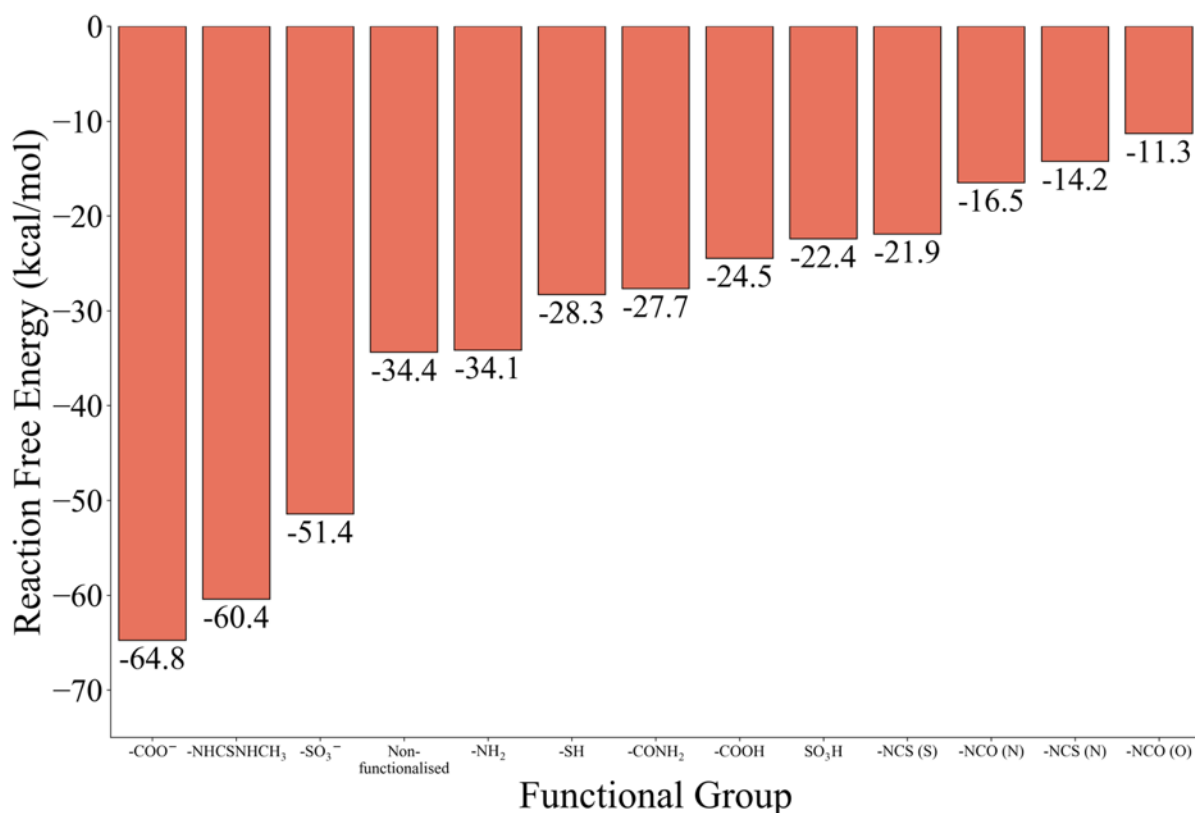


Figure S2. Comparison of the reaction free energy (ΔG) in kcal/mol of the lone Pb^{2+} ion binding onto different adsorption sites on functionalised linkers (labelled according to the functional group for brevity) with no water molecules present. The reaction plotted is $Pb^{2+} + L^n \rightarrow L-Pb^{n+2}$ where L is the functionalised MOF and $n=0$ for all ligands except COO^- and SO_3^- where $n=1$. For the -NCS and -NCO functionalised MOFs, the atom in brackets is the adsorption site where Pb^{2+} is bound.

Unlike the reaction depicted in Fig. 4 of the main text which is an exchange reaction between water and the functionalised linkers, the reaction in Fig. S2 is direct adsorption of fully desolvated Pb^{2+} with no loss or gain of water molecules (comparable to Fig. 5 in the main text, which examines adsorption of partially desolvated Pb^{2+}). As described in the main text, the notation for functionalised UiO-66 is simply the functional group that acts as the adsorption site (*i.e.*, UiO-66-SH is reported as -SH). Not surprisingly, the ΔG s are all consistently and significantly more favourable relative to those found when modelling solvated Pb^{2+} adsorption using explicit water molecules but the overall adsorption trend remain similar. Charged ($-COO^-$, $-SO_3^-$) and chelating ($-COO^-$, $-NHCSNHCH_3$) species are still the most favourable, with the ΔG of Pb^{2+} adsorbing onto $-COO^-$ equal to -64.8 kcal/mol (in close agreement with density functional theory calculations conducted by Zhao *et al.*^[15]). However, we observe that the -SH functional group now demonstrates more favourable ΔG s compared to the $-CONH_2$ functional

group once all explicit water molecules are removed. Note that in the absence of the explicit solvation shell the coordination geometry spontaneously optimised to a chelating geometry for both of these functional groups. The significant steric strain caused by the proximity of the two functional groups in $-\text{CONH}_2$ leads to this adsorption configuration being less favourable than $-\text{SH}$. In addition to these trends, we found that we were able to stabilize a greater variety of geometries during the optimization process in the absence of explicit water molecules. In particular, we successfully optimized geometries with Pb^{2+} bound to the nitrogen atom rather than the terminal oxygen and sulphur atoms for the $-\text{NCO}$ and $-\text{NCS}$ ligands, respectively. The steric bulk introduced when incorporating a partial or full solvation shell clearly prevents adsorption on less accessible binding sites. This suggests that if Pb^{2+} is partially or fully desolvated as it passes through the triangular aperture, it could potentially interact with more sites on functionalised linkers.

5) Effect of water cluster size and model chemistry on Pb^{2+} solvation free energies

In the main text we thoroughly discussed our choice of model chemistry and coordination number for solvated Pb^{2+} based on consistency with experimental findings reporting a hemidirected geometry with bond lengths comparable to our $\text{Pb}(\text{H}_2\text{O})_6^{2+}$ simulated complex. Another way to validate our computational method is by comparing computed solvation free energies to the experimental literature. In addition to the water cluster size, we considered the functional and basis set used for the calculations.

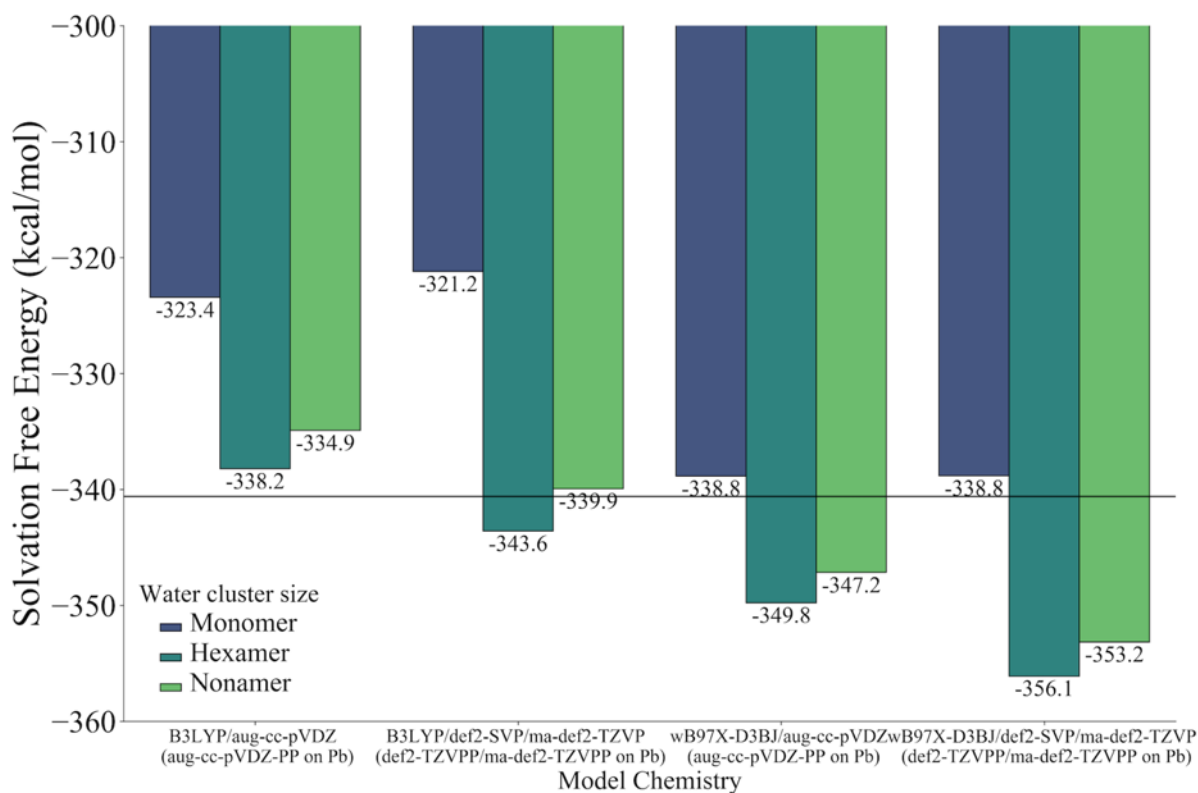


Figure S3. Comparison of Pb^{2+} solvation free energy computed using different combinations of two functionals (B3LYP and ω B97X-D3BJ) and two basis set (aug-cc-pVDZ (aug-cc-pVDZ-PP on Pb) and def2-SVP/ma-def2-TZVP (def2-TZVPP/ma-def2-TZVPP on Pb)). Solvation free energies were calculated according to Eqn. S1 and by modelling six explicit water molecules coordinating solvated Pb^{2+} . Three water cluster sizes are considered to model the solvent molecules: a monomer, a hexamer, and a nonamer. The experimental solvation free energy of the Pb^{2+} ion (-340.6 kcal/mol)^[16] is depicted as a black line.

We calculated the solvation free energy according to Eqn. S1 with $n=6$ (i.e., modelling $Pb^{2+}_{(g)} + 6H_2O_{(aq)} \rightarrow Pb(H_2O)_6^{2+}_{(aq)}$) using four combinations of functionals (B3LYP^[17] and ω B97X-D3BJ^[12,13]) and basis sets (aug-cc-pVDZ (aug-cc-pVDZ-PP with the SK MCDHF RSC ECP on Pb)^[5-7,18] and def2-SVP/ma-def2-TZVP (def2-TZVPP/ma-def2-TZVPP with the def2- ECP on Pb)^[7-9]) (Fig. S3). Of all possible combinations of basis sets and functionals presented in Table 1 in the main text, here we focus on these four combinations based on previous literature. Both selected functionals had previously been used for modelling Pb^{2+} solvation shells;^[2,3] the basis sets were chosen either because they have been recommended in the literature for Pb^{2+} hydration (in the case of aug-cc-pVDZ (aug-cc-pVDZ-PP with the SK MCDHF RSC ECP on Pb))^[2,3] or because they have been used previously by us to model heavy metal adsorption on UiO-66 (def2-SVP/ma-def2-TZVP (def2-TZVPP/ma-def2-TZVPP with the def2- ECP on

Pb)).^[19] B3LYP generates solvation free energies less negative than ω B97X-D3BJ across all basis sets and water cluster sizes, with the B3LYP/def2-SVP/ma-def2-TZVP (def2-TZVPP/ma-def2-TZVPP with the def2-ECP on Pb) model chemistry producing the closest solvation free energy to experimental values (-339.9 kcal/mol calculated vs. -340.6 kcal/mol experimental^[16]). However, as previously noted, the use of B3LYP always leads to holodirected geometries (Table 1 in the main text and related discussion) that are in disagreement with the experimental literature,^[14] and hence this functional is not a good choice to accurately model solvated Pb^{2+} . The basis set effect on the computed solvation free energy is less significant compared to the functional effect. We do observe however that the aug-cc-pVDZ basis set consistently produces solvation free energies less negative than the def2 series of basis sets and closer to the experimental value. Overall, the trends indicate that our chosen model chemistry (ω B97X-D3BJ/def2-SVP/ma-def2-TZVP (def2-TZVPP/ma-def2-TZVPP with the def2-ECP on Zr, Pb)) could potentially slightly overestimate solvation free energies. However, solvation free energies are only one way to benchmark a model chemistry and our chosen computational method is backed by numerous benchmark studies reported in the main text and in the literature.^[20–22] Furthermore, this is the same method we used in our previous study in which we developed a cluster model for the UiO-66 nodes, which we employ in the current study to model Pb^{2+} interaction with defect sites.^[19]

The size of the water cluster also has a non-negligible effect on the computed solvation free energies (Fig. S3), with the ordering of accuracy relative to the experimental value (-340.6 kcal/mol) being the monomer (-338.8 kcal/mol), followed by the nonamer (-353.2 kcal/mol) and hexamer (-356.1 kcal/mol) when using our selected model chemistry. As discussed previously, this is an artifact of our model chemistry overestimating solvation free energies relative to the experimental value combined with the fact that the monomer provides less thermodynamic driving force for solvation of Pb^{2+} to occur. Given that the choice of functional

and basis set plays a significant role (as demonstrated by Fig. S3), the use of a larger water cluster such as a nonamer to describe free water remains the most suitable choice. This choice is also consistent with our previous study on As(V) adsorption by UiO-66.^[19]

6) Effect of adsorbed Pb²⁺ coordination number and water cluster size on reaction free energies

We assessed the effect of the coordination number of adsorbed Pb²⁺ and the water cluster size on the reaction free energies (ΔG s) by using the adsorption of Pb(H₂O)₆²⁺ onto UiO-66-NH₂ as a case study. We chose this adsorption site as it was the most stable adsorption site on functionalised linkers without confounding factors such as chelation (where higher coordination numbers could impose steric strain on the structure) or electrostatic attraction (as the Pb²⁺ cation becomes less electrophilic when coordinated by additional water molecules). This analysis was done on two types of reactions: the exchange of a water molecule with a functionalised linker (*i.e.*, Pb²⁺ coordination number constant and equal to six across the reaction) and direct adsorption with no loss or gain of free water molecules (*i.e.*, final coordination number seven). The reaction with a final coordination number of seven is more favourable than six, likely since Pb²⁺ is not forced to lose a coordinated water molecule and is stabilized by the increased number of bonds; this agrees with our observation in Fig. 2 that Pb(H₂O)₇²⁺ is the most stable solvated Pb²⁺ species. That said, the ΔG differences between coordination numbers are very small (2.3 kcal/mol at most), hence both final complexes are likely thermodynamically accessible at room temperature. With regards to the water cluster size, the ΔG differences are mostly negligible (less than 2 kcal/mol with the largest difference being between the monomer and the hexamer). This further corroborates our choice for modelling solvating water using a nonamer cluster as it shows that our predicted ΔG s for Pb²⁺ adsorption are not dramatically affected by the choice of water cluster size.

Table S2. Comparison of the reaction free energy (ΔG) in kcal/mol for the $Pb(H_2O)_6^{2+}$ complex adsorbing onto UiO-66-NH₂ with different final coordination numbers and different water cluster sizes used to model the product water molecule. The reaction considered is $Pb(H_2O)_6^{2+} + UiO-66-NH_2 \rightarrow UiO-66-NH_2-Pb(H_2O)_a^{2+} + bH_2O$, where a is the final coordination number -1, and $b=0$ for final coordination number 7 and 1 for final coordination number 6. Note that the ΔG for coordination number 7 is identical across water cluster size as there are no water molecules involved in the reaction.

Final coordination number	Final species	Monomer	Hexamer	Nonamer
6	UiO-66-NH ₂ -Pb(H ₂ O) ₅ ²⁺	5.3	6.9	6.4
7	UiO-66-NH ₂ -Pb(H ₂ O) ₆ ²⁺	4.6	4.6	4.6

7) Cartesian coordinates of gas-phase optimized structures

For the reader's convenience, the geometries are organised according to the figure in which data based on each geometry is first presented. If the model chemistry was not specified, the model chemistry used for the geometry optimization was $\omega B97X-D3BJ/def2-SVP$ (def2-TZVPP with def2- ECP on Pb).

Main text:

Fig. 1

Holodirected $Pb(H_2O)_6^{2+}$ calculated with B3LYP/def2-SVP (def2-TZVPP with def2- ECP on Pb)

O	1.43637985787516	1.81297290474298	-3.05311474676010
H	1.38262597990187	1.89906293283224	-4.02014572007958
H	1.87012435077244	2.63128644234749	-2.75564840975884
Pb	-0.18988926582389	0.40104921990115	-1.56018945183805
H	2.13945085453817	-1.70539326054306	-1.61922977362471
O	1.90650493420354	-0.79352571852397	-1.85997658747895
H	2.62900745674803	-0.42491473557606	-2.39563900426673
H	-1.04535450067407	-2.58318836370883	-0.83177584809120
O	-0.59409020756623	-1.82633646734635	-0.42173361678340
H	-0.60025743041227	-1.99935704490811	0.53495495915600
H	-3.83267593542388	0.39348603082584	-2.53491959176907
O	-2.99750822181821	0.73200633123124	-2.90049267689440
H	-3.26555786930266	1.52072157398912	-3.40220259432037
H	-1.87393660330951	-0.48118263211827	-3.68652277723310
O	-0.97771835343896	-0.85683221800309	-3.52527334795881
H	-0.70824335678746	-1.39979810010245	-4.28266592429507
H	2.00416105551526	0.72370273053508	0.85823781812588
O	1.11323085146045	1.01678977936432	0.60521202866352
H	0.82259640354223	1.59795059506073	1.32905526520735

Hemidirected $Pb(H_2O)_6^{2+}$ calculated with $\omega B97X-D3BJ/def2-SVP$ (def2-TZVPP with def2- ECP on Pb)

O	0.46125686648664	2.66521291489378	-2.78376694134932
H	0.64524705960750	3.07492028137945	-3.64276009137161
H	0.81811945582891	3.29153901456616	-2.13665825177748
Pb	0.33176752909928	0.01495812450161	-2.32414451910685
H	3.39767823445672	-0.73349131538071	-1.25558509349437
O	2.48721771185152	-0.98188454904932	-1.03424354136660
H	2.55524080010292	-1.90100033427495	-0.73515624768849
H	-1.34442387557520	-2.31983608250894	-1.99190834527032
O	-0.87080749108760	-1.83874350110906	-1.29295652595119
H	-1.11282921635467	-2.21006708149811	-0.43361768076606
H	-1.70227431035718	2.15269124172192	-2.27983062591454
O	-1.76922211740369	1.22194281105631	-2.01481579934374
H	-2.67156943457437	1.05423277776687	-1.70925629970422
H	-2.04624878063766	-1.29885205944685	-4.35457432616580
O	-1.21308873951647	-1.58604714126481	-3.95213562656478
H	-0.83234593864221	-2.19521751322020	-4.60321255236138

H	1.40647552964882	0.36364014911603	0.38532310868759
O	0.61590424620662	0.74674493404379	-0.02657209618736
H	0.06275247086015	1.13775732870703	0.66380145569712

Table 1

Pb(H₂O)₆²⁺ calculated with PBE0/def2-SVP (def2-SVP with def2- ECP on Pb)

O	0.46125686648664	2.66521291489378	-2.78376694134932
H	0.64524705960750	3.07492028137945	-3.64276009137161
H	0.81811945582891	3.29153901456616	-2.13665825177748
Pb	0.33176752909928	0.01495812450161	-2.32414451910685
H	3.39767823445672	-0.73349131538071	-1.25558509349437
O	2.48721771185152	-0.98188454904932	-1.03424354136660
H	2.55524080010292	-1.90100033427495	-0.73515624768849
H	-1.34442387557520	-2.31983608250894	-1.99190834527032
O	-0.87080749108760	-1.83874350110906	-1.29295625295119
H	-1.11282921635467	-2.21006708149811	-0.43361768076606
H	-1.70227431035718	2.15269124172192	-2.27983062591454
O	-1.76922211740369	1.22194281105631	-2.01481579934374
H	-2.67156943457437	1.05423277776687	-1.70925629970422
H	-2.04624878063766	-1.29885205944685	-4.35457432616580
O	-1.21308873951647	-1.58604714126481	-3.95213562656478
H	-0.83234593864221	-2.19521751322020	-4.60321255236138
H	1.40647552964882	0.36364014911603	0.38532310868759
O	0.61590424620662	0.74674493404379	-0.02657209618736
H	0.06275247086015	1.13775732870703	0.66380145569712

Pb(H₂O)₆²⁺ calculated with PBE0/def2-SVP (def2-SVP with def2- ECP on Pb)

O	0.17529784069660	2.84061147074175	-2.93571479390944
H	0.20392391209280	3.15363623281688	-3.85272251490026
H	0.56041116384083	3.57001742748579	-2.42751880286804
Pb	0.37098452228263	0.02870187863945	-2.24651361482112
H	3.34429502886333	-1.04068199863470	-1.22021772429402
O	2.40857020433705	-1.19485286892367	-1.01960449302888
H	2.36560423249571	-2.12634745132420	-0.75621395707436
H	-1.27033396652513	-2.34410027413173	-1.90611400849208
O	-0.75413707195290	-1.83940234894448	-1.25757691190408
H	-1.09121081444339	-2.02960585899049	-0.37080038530354
H	-1.48735640391104	2.13931388148533	-2.32057871637871
O	-1.70064936886255	1.23310590207299	-2.02262761571571
H	-2.59433022698272	1.20710244788552	-1.65511151117887
H	-1.85647805870627	-1.20525840907595	-4.35469207316522
O	-1.03350882306276	-1.50571795773414	-3.94113664478559
H	-0.62229733636747	-2.07853395870758	-4.60669201226971
H	1.40424130711582	0.16673954719892	0.49224919708029
O	0.59001577055663	0.53703614966172	0.11702671347780
H	0.20580808853284	1.14673618847860	0.76248986953219

Pb(H₂O)₆²⁺ calculated with PBE0/aug-cc-pVDZ (aug-cc-pVDZ-PP with SK MCDHF-RSC ECP on Pb)

O	1.34815410532497	1.83388367060681	-3.32878875353066
H	1.31695555320122	1.87037973506648	-4.29378129502067
H	1.78121164120733	2.65589525047465	-3.06279293635117
Pb	-0.17877293438965	0.28211468242410	-1.83834696248294
H	2.28601040126165	-1.79701459075108	-1.63641304409057
O	2.02160174144426	-0.94828727764475	-2.01336896010443
H	2.80462993362442	-0.58336969990158	-2.44533128890144
H	-1.21761441971648	-2.62441627966118	-0.82316002232578
O	-0.76094803541043	-1.82554084520538	-0.52885116285670
H	-0.72010175255181	-1.88409737389918	0.43479861115448
H	-3.46882847418423	0.81842087413202	-1.57467967406024
O	-2.67988950832623	1.19139037075141	-1.98891852852746
H	-2.97373056783657	2.03088137547626	-2.36617913487303
H	-1.54553274168029	-1.02015226001794	-4.44537388528519
O	-0.72329725598647	-1.06525536863812	-3.93997654764231
H	-0.17829661165154	-1.73087202248389	-4.37945394974903
H	1.43203965740161	0.85360917826872	0.97839822003041
O	0.56404968781734	0.98638543856421	0.57590532718532
H	0.11120958045087	1.61454514243841	1.15424398743175

Pb(H₂O)₆²⁺ calculated with B3LYP/def2-SVP (def2-SVP with def2- ECP on Pb)

O	1.43637985787516	1.81297290474298	-3.05311474676010
H	1.38262597990187	1.89906293283224	-4.02014572007958
H	1.87012435077244	2.63128644234749	-2.75564840975884
Pb	-0.18988926582389	0.40104921990115	-1.56018945183805
H	2.13945085453817	-1.70539326054306	-1.61922977362471

O	1.90650493420354	-0.79352571852397	-1.85997658747895
H	2.62900745674803	-0.42491473557606	-2.39563900426673
H	-1.04535450067407	-2.58318836370883	-0.83177584809120
O	-0.59409020756623	-1.82633646734635	-0.42173361678340
H	-0.60025743041227	-1.99935704490811	0.53495495915600
H	-3.83267593542388	0.39348603082584	-2.53491959176907
O	-2.99750822181821	0.73200633123124	-2.90049267689440
H	-3.26555786930266	1.52072157398912	-3.40220259432037
H	-1.87393660330951	-0.48118263211827	-3.68652277723310
O	-0.97771835343896	-0.85683221800309	-3.52527334795881
H	-0.70824335678746	-1.39979810010245	-4.28266592429507
H	2.00416105551526	0.72370273053508	0.85823781812588
O	1.11323085146045	1.01678977936432	0.60521202866352
H	0.82259640354223	1.59795059506073	1.32905526520735

Pb(H₂O)₆²⁺ calculated with B3LYP/def2-SVP (def2-TZVPP with def2- ECP on Pb)

O	1.06173233406008	2.06014554323765	-3.16607752305032
H	1.01356229209417	2.23733549388404	-4.12053331995537
H	1.54650958879414	2.81534251873179	-2.79322628768656
Pb	-0.06247845311586	0.09645780234780	-1.87775909081077
H	2.40975341892827	-2.02893651045247	-1.67023033647995
O	2.17007130255316	-1.17510527375562	-2.06744191030547
H	2.98528423949678	-0.84287517118472	-2.47939639604554
H	-1.33400068377098	-2.70134444656966	-0.74934205712916
O	-0.95482578242646	-1.85397842369260	-0.46189756911434
H	-1.04739192523158	-1.84497815098715	0.50562728835806
H	-3.24477411409383	0.82503332516520	-1.55023878763190
O	-2.43475398600187	1.16949242237880	-1.96230888818555
H	-2.68523929714199	2.03324933571317	-2.33081071292965
H	-1.49160524090440	-1.12665736114735	-4.52703029741536
O	-0.66005922333266	-1.17524944477718	-4.02607500332247
H	-0.09531520444030	-1.79403397094712	-4.51884567267675
H	1.37296736238693	0.97704845458426	0.94904566549117
O	0.56577015171210	1.13428643999864	0.43086631916992
H	0.10364322043429	1.85326741747249	0.89360457972029

Pb(H₂O)₆²⁺ calculated with B3LYP/aug-cc-pVDZ (aug-cc-pVDZ-PP with SK MCDHF-RSC ECP on Pb)

O	1.05755622006220	2.03514834378311	-3.22239698137472
H	1.04597115126299	2.16486844468625	-4.18307400278943
H	1.51249243440152	2.81247074165283	-2.86358309334232
Pb	-0.07636333383996	0.06786854769645	-1.89992079506696
H	2.498268688930228	-1.94721864382618	-1.53814293018261
O	2.26374972870708	-1.07998058325897	-1.90253236292587
H	3.06718764247149	-0.75205107544243	-2.33505918289766
H	-1.38175362375682	-2.74367623574355	-0.76490584106605
O	-0.96980799304152	-1.91784134647423	-0.46755403562650
H	-0.99001320445243	-1.95041502369019	0.50112308278294
H	-3.26097948687638	0.85987582879073	-1.50116104896434
O	-2.45480957015694	1.19940806610529	-1.91900358625183
H	-2.70139110023598	2.05876041733097	-2.29403156434658
H	-1.58921786353098	-1.10277085373969	-4.57243988356396
O	-0.74436591908887	-1.17758519247786	-4.10241889089977
H	-0.21645867840273	-1.80791532487308	-4.61640170090761
H	1.43987099140409	1.00332426527471	0.85958390221224
O	0.59838345592327	1.13142866547408	0.39568157428419
H	0.12053045984770	1.80480095873177	0.90416734092709

Pb(H₂O)₆²⁺ calculated with B3LYP_D3BJ/def2-SVP (def2-TZVPP with def2- ECP on Pb)

O	1.66119869166044	1.94864340313664	-3.01730896225309
H	1.81798044506875	2.29060026924060	-3.91410149785959
H	1.96851873716893	2.65398698958579	-2.42317565294215
Pb	-0.22630261011458	0.24367686932787	-2.30870983831227
H	2.33993740686343	-1.53344408919393	-1.63797775987360
O	2.00295147137354	-0.69303106551077	-1.98830929250107
H	2.75573231876391	-0.18468350971637	-2.33483486387278
H	-1.03920452021112	-2.43778767170361	-1.74662779551746
O	-0.78319482840290	-1.78754637802031	-1.06275043319017
H	-1.02528794952666	-2.12965592589402	-0.18776161843729
H	-3.07478091877602	1.19015150386275	-0.73351070444440
O	-2.28514139084359	1.60494995112618	-1.12109553003266
H	-2.60475871416815	2.45991821462726	-1.45815534605352
H	-1.73592635986117	-2.20913550329761	-4.23775155564759
O	-0.91290073328449	-2.13178824800381	-3.72450286345435
H	-0.28101321257712	-2.69670428679329	-4.20182147880860

H	0.90249697476114	1.11170729493326	0.54734831486468
O	0.26772475076089	1.26856888500588	-0.17042313508224
H	-0.52917955865523	1.69007329728750	0.19940001341848

Pb(H₂O)₆²⁺ calculated with ω B97X/def2-SVP (def2-TZVPP with def2- ECP on Pb)

O	1.31388230155041	2.32284645738334	-2.89527562743578
H	1.53429070747097	2.70269494816166	-3.75858011048773
H	1.56431068289797	2.99521380366766	-2.24597628723232
Pb	0.02766311232409	0.15326970472692	-2.38744654714967
H	2.58912197879588	-1.51893289769693	-1.27323970469360
O	2.34765685126594	-0.62087783206101	-1.54444609569406
H	3.15835526420868	-0.24420512933980	-1.91892743685708
H	-1.29822097630107	-2.25560234616988	-1.74654307701095
O	-0.95314953117071	-1.64706187735046	-1.06196117463489
H	-1.08587310619886	-2.03545287093804	-0.18750715408533
H	-2.82799543584754	1.02438662895274	-1.31124269229448
O	-2.06071727906039	1.41746518590254	-1.75262928392079
H	-2.37340021203059	2.25746310994538	-2.12023294213678
H	-2.25725021326747	-2.13569439381821	-4.02023351111656
O	-1.37974623711135	-2.19207743088865	-3.61380292340195
H	-0.93952737744301	-2.90007775959695	-4.10735340723672
H	1.34043654512071	0.75398037377550	0.22216129741690
O	0.54090678103394	1.06933968465001	-0.22484109176831
H	-0.02189385623761	1.51182264069422	0.42600776974036

Pb(H₂O)₆²⁺ calculated with ω B97X-D3BJ/def2-SVP (def2-SVP with def2- ECP on Pb)

O	0.48436680906779	2.68217391888342	-2.76264144669216
H	0.62898138898407	3.12613987202189	-3.61327907834367
H	0.84645417898307	3.29323116922769	-2.10217608267823
Pb	0.35848772158266	0.02333562055308	-2.37080248949193
H	3.37364268095075	-0.83273681930094	-1.28590272641397
O	2.44811593892174	-1.04790560016935	-1.08771831597572
H	2.47604091687355	-1.96481469941666	-0.77202700933375
H	-1.31484710208239	-2.35155094689463	-1.90590161633640
O	-0.82688454049927	-1.80987051292678	-1.26418791375977
H	-1.02725973331723	-2.13388109984978	-0.37418067082054
H	-1.73289570739376	2.13045172833462	-2.25112942504163
O	-1.76631298033505	1.19051397206361	-2.01114245652850
H	-2.66885205929787	0.97976823660239	-1.73042982889996
H	-2.03002607623927	-1.28999168973194	-4.34481804196152
O	-1.18015373280914	-1.55925347831075	-3.96230217737900
H	-0.80199862496229	-2.16091051688397	-4.62389751657778
H	1.35809087725434	0.41497072730465	0.41062481983148
O	0.58514247612987	0.76773413801214	-0.05829409042372
H	0.00875756818843	1.20109598048131	0.58813606682736

Pb(H₂O)₆²⁺ calculated with ω B97X-D3BJ/def2-SVP (def2-TZVPP with def2- ECP on Pb)

O	0.46125686648664	2.66521291489378	-2.78376694134932
H	0.64524705960750	3.07492028137945	-3.64276009137161
H	0.81811945582891	3.29153901456616	-2.13665825177748
Pb	0.33176752909928	0.01495812450161	-2.32414451910685
H	3.39767823445672	-0.73349131538071	-1.25558509349437
O	2.48721771185152	-0.98188454904932	-1.03424354136660
H	2.55524080010292	-1.90100033427495	-0.73515624768849
H	-1.34442387557520	-2.31983608250894	-1.99190834527032
O	-0.87080749108760	-1.83874350110906	-1.29295652595119
H	-1.11282921635467	-2.21006708149811	-0.43361768076606
H	-1.70227431035718	2.15269124172192	-2.27983062591454
O	-1.76922211740369	1.22194281105631	-2.01481579934374
H	-2.67156943457437	1.05423277776687	-1.70925629970422
H	-2.04624878063766	-1.29885205944685	-4.35457432616580
O	-1.21308873951647	-1.58604714126481	-3.95213562656478
H	-0.83234593864221	-2.19521751322020	-4.60321255236138
H	1.40647552964882	0.36364014911603	0.38532310868759
O	0.61590424620662	0.74674493404379	-0.02657209618736
H	0.06275247086015	1.13775732870703	0.66380145569712

Pb(H₂O)₆²⁺ calculated with ω B97X-D3BJ/aug-cc-pVDZ (aug-cc-pVDZ-PP with SK MCDHF-RSC ECP on Pb)

O	0.70235058370255	2.58272856884130	-2.71894320352849
H	0.91204636499566	3.05653681988316	-3.53589127224653
H	1.00021158388945	3.16318727668260	-2.00540771530934
Pb	0.32842304857748	0.00155467199481	-2.37773316603792
H	3.41901232010605	-0.74425500284330	-1.38831951113783
O	2.51346487861733	-1.01919628156189	-1.18652103118814

H	2.60143787852442	-1.92477223748917	-0.85825005685767
H	-1.42052673951065	-2.41251071760418	-1.74413265563679
O	-0.97559547412999	-1.75965713847384	-1.18559734920464
H	-0.99463941243779	-2.09572289157888	-0.28005527276022
H	-2.04839073970287	2.01993346242653	-2.28083464010086
O	-1.86700590093179	1.11178595394632	-2.00254556518077
H	-2.69931680089368	0.73839700248394	-1.68430829806381
H	-2.03429936138919	-1.19942637871697	-4.42962305777315
O	-1.19013747408791	-1.48730519162447	-4.05636392399885
H	-0.83182243204495	-2.10229788495606	-4.71199762735235
H	1.31973139745204	0.58947293494969	0.46775776735823
O	0.56118466523830	0.86044623395771	-0.06765629994768
H	-0.07727838597444	1.27960079968271	0.52435287896741

Pb(H₂O)₆²⁺ calculated with ωB97X-D3BJ/def2-SVP (LANL2DZ with HayWadt ECP on Pb)

O	0.46109634929255	2.65231679334236	-2.63406418878261
H	0.61111311815923	3.14409398442413	-3.45758783024643
H	0.84198744833871	3.21310346757742	-1.94023465057611
Pb	0.39565641480453	0.03509647679215	-2.44100366652185
H	3.29372395679949	-0.92135602628905	-1.31126837744665
O	2.35724458136552	-1.08686826665253	-1.11470182786710
H	2.33855041546726	-1.99677956784798	-0.77824908744016
H	-1.26717089923311	-2.25915494600052	-1.84578160936799
O	-0.77542049539056	-1.65562811771787	-1.26422364967674
H	-0.91557474153080	-1.92126291271774	-0.34348557937199
H	-1.72222764906652	2.03094270088739	-2.23782021448627
O	-1.69343203759103	1.08059662210989	-2.03884046429441
H	-2.58205126403892	0.78685422044670	-1.78882396631684
H	-2.02471895411693	-1.26676001020257	-4.30431150163981
O	-1.17246471134508	-1.53270729216261	-3.92445787170040
H	-0.80695371274801	-2.15533272764127	-4.57403761753605
H	1.33133370535379	0.46067058897629	0.30265097441935
O	0.57856398525736	0.79542228871083	-0.21132777050547
H	-0.03040550977748	1.25525272396496	0.38549889935813

Pb(H₂O)₆²⁺ calculated with ωB97X-D3BJ/6-31G(d,p) (LANL2DZ with HayWadt ECP on Pb)

O	0.46797184980072	2.64814843446997	-2.63241106618031
H	0.65266545516041	3.15497844475943	-3.43593127231586
H	0.86423223284674	3.15543284058116	-1.91044157128779
Pb	0.38475848321651	0.04859513105622	-2.44055894880530
H	3.27505827996739	-0.90340253885693	-1.31515787275317
O	2.34068087982970	-1.05515120499043	-1.11190611792878
H	2.29638655538584	-1.97058619569111	-0.80218477240932
H	-1.25502111992279	-2.24445393396069	-1.89041786258354
O	-0.74720979413933	-1.69288055514541	-1.27555252902766
H	-0.95375478934341	-1.94988849652030	-0.36822792792289
H	-1.70487282551363	2.05058048503926	-2.18297614534908
O	-1.68824986895429	1.11255114628602	-1.94202931440063
H	-2.59337184720005	0.80729440452859	-1.79999349829981
H	-2.02462898286024	-1.32005858673199	-4.34067010947040
O	-1.19045568266940	-1.57406176411200	-3.92182140629852
H	-0.79436036108809	-2.20917945237324	-4.53603477054294
H	1.33587146248408	0.49272263768776	0.26987387210468
O	0.61417386112143	0.88415827940799	-0.24364896884059
H	-0.06102378812159	1.22370092456570	0.35802028231254

Fig. 2

<u>Pb(H₂O)²⁺</u>			
Pb	0.27613390767502	0.08632344362394	-2.25332002695165
H	1.44157244124602	0.41448258761067	0.47764340978302
O	0.64927505711891	0.63056134390731	-0.06034475886370
H	0.04991859396005	1.13173262485809	0.53443137603233

<u>Pb(H₂O)₆²⁺</u>			
O	0.55422652744435	2.54258878861922	-2.70804407706179
H	0.18756319976690	2.99607432679756	-3.49358743321384
H	1.00968689053717	3.23293201775986	-2.18753760865715
Pb	0.58409769998366	0.24188928615081	-2.36818809186478
H	1.11856194494837	0.15578108508333	0.58138673701487
O	0.69078479084474	0.72187291996107	-0.09219918801208
H	0.19660894647480	1.40363157562813	0.40338966179477

<u>Pb(H₂O)₆²⁺</u>			
O	1.06123002239061	2.03669786753196	-2.57495285862920

H	1.12644438903985	2.37661611945483	-3.48678262613604
H	1.21504839947736	2.79831797281630	-1.98726019301016
Pb	0.12706085841670	-0.02973703950120	-1.91296982331086
H	3.15525093956982	-0.11022992076175	-1.88027776021529
O	2.38905300308592	-0.63395935973774	-1.58361257851957
H	2.72302129118580	-1.53483609068579	-1.41521530854687
H	1.07317249120666	0.71318152891009	0.86507600837735
O	0.32249343654779	0.87126327915760	0.26438353169118
H	-0.41110483092052	1.19108564281570	0.82184160829949

Pb(H₂O)₆²⁺

O	1.05900852350194	2.09888318585848	-2.68761862280922
H	1.29430337815463	2.43541854600205	-3.56997524070440
H	1.31705162467579	2.78512062193649	-2.04928445125967
Pb	0.13290801733333	-0.03288913429908	-2.14144341598666
H	3.26501269978608	-0.07754748184708	-1.58407662077244
O	2.45757171004183	-0.58543828081500	-1.39901703929061
H	2.76356735133534	-1.49692971140599	-1.25044633659316
H	-2.00866360438572	2.24959334927686	-2.06946628949433
O	-1.90092839060629	1.33330839029102	-1.77225337263871
H	-2.79787507219998	0.96969847666670	-1.67437969383613
H	1.09669502604004	0.53795187953921	0.63108595081101
O	0.34558924996830	0.76619526525081	0.05766656915891
H	-0.36563051364531	1.12389489354550	0.61552856341546

Pb(H₂O)₆²⁺

O	0.99912959084948	2.41511755545611	-2.59488832455809
H	1.27774969016648	2.85392350157542	-3.41516006846973
H	1.22514743655781	3.02955250259659	-1.87972969786368
Pb	0.21691879717966	0.03746111816023	-2.37226609772220
H	3.30594916233759	-0.38020423283869	-1.61216521864063
O	2.44393279972747	-0.73922373815809	-1.34529772785342
H	2.62717436737938	-1.65812660729004	-1.09002246537586
H	-1.24298579785815	-2.69351823885401	-1.68130777305372
O	-0.93801210660809	-1.88695800745104	-1.23443349760125
H	-1.12745212975614	-2.02646683999069	-0.29375739940875
H	-2.05190304297822	2.16865520103924	-2.18016001068286
O	-1.89232458648925	1.26740410604828	-1.85647818949240
H	-2.76963917914284	0.85929611180982	-1.77601496193420
H	1.14963489079789	0.54544956701479	0.43074463639223
O	0.37946665336709	0.74824698798180	-0.12346524343002
H	-0.29223654553018	1.19800101290027	0.41223203969464

Pb(H₂O)₆²⁺

O	0.46125686648664	2.66521291489378	-2.78376694134932
H	0.64524705960750	3.07492028137945	-3.64276009137161
H	0.81811945582891	3.29153901456616	-2.13665825177748
Pb	0.33176752909928	0.01495812450161	-2.32414451910685
H	3.39767823445672	-0.73349131538071	-1.25558509349437
O	2.48721771185152	-0.98188454904932	-1.03424354136660
H	2.55524080010292	-1.90100033427495	-0.73515624768849
H	-1.34442387557520	-2.31983608250894	-1.99190834527032
O	-0.87080749108760	-1.83874350110906	-1.29295652595119
H	-1.11282921635467	-2.21006708149811	-0.43361768076606
H	-1.70227431035718	2.15269124172192	-2.27983062591454
O	-1.76922211740369	1.22194281105631	-2.01481579934374
H	-2.67156943457437	1.0542327776687	-1.70925629970422
H	-2.04624878063766	-1.29885205944685	-4.35457432616580
O	-1.21308873951647	-1.58604714126481	-3.95213562656478
H	-0.83234593864221	-2.19521751322020	-4.60321255236138
H	1.40647552964882	0.36364014911603	0.38532310868759
O	0.61590424620662	0.74674493404379	-0.02657209618736
H	0.06275247086015	1.13775732870703	0.66380145569712

Pb(H₂O)₆²⁺

Pb	-0.04814467811420	0.09239181945155	-0.14804064358735
O	-0.45682176577398	-2.37714974967581	0.06993649213991
H	-1.32597791320002	-2.51141613570511	-0.34634303713235
H	-0.18547687218929	-3.21368253468384	0.47165910357774
O	1.50179046577672	2.26773289455020	0.13052859751816
H	2.13519926161030	2.18538549777799	0.85946993127053
H	1.88558889990626	2.91385584591577	-0.48159793857557
O	-2.49310045003839	-1.00166897714289	-1.15383647903906
H	-2.64555114514599	-1.07299423436128	-2.10924686465187
H	-3.38208474670313	-0.90611648336028	-0.78008820988570

O	-1.18249880012143	0.03743380266140	2.04678302009957
H	-1.67731101037054	-0.63555474929622	2.53473589719730
H	-1.61083949004553	0.89745683014575	2.19166157138094
O	1.65892851894370	-0.18955503863973	1.59699829119061
H	1.48738964904135	-0.43874419791599	2.51716409491123
H	2.41143470378597	-0.71181549397992	1.27499789557338
O	2.27031739676293	-1.03032954480168	-0.97216670170647
H	2.26610250998236	-1.93825300433522	-1.31157559540959
H	2.96974853653290	-0.58639880562746	-1.47587404773281
O	-1.31930315756740	2.34357938017062	0.59157785114107
H	-0.60718829578339	2.99946001768960	0.65914563700950
H	-2.10626961728920	2.83054686116255	0.30482613471079

Pb(H₂O)₈²⁺

Pb	0.00442777345440	0.02073567485086	-0.00787883213185
O	-1.79173142933752	1.35452693096900	-1.47551019185600
H	-2.28348559198065	0.61969030761097	-1.87727404897300
H	-1.87029205936929	2.10691180578874	-2.07963387593626
O	1.79344871149286	1.94344944943981	0.40226000391400
H	2.28891814532937	1.93182424313177	-0.43302628660392
H	1.81321247890718	2.85436710731868	0.72933949823532
O	-1.70951916717653	-1.36348274641783	1.47896291006271
H	-2.22557265681477	-0.66179852710012	1.90830713601848
H	-1.73422263944122	-2.12674626096529	2.07408566545530
O	1.79705127557771	0.41952812751619	-1.94137209975328
H	1.80663341913997	0.74029512690457	-2.85480979965635
H	2.28952154051434	-0.41732390691889	-1.93452469973631
O	1.74180606214656	-0.40215020829568	1.94312517806798
H	2.26447869141064	0.41645837409395	1.94605096528934
H	1.73176745236258	-0.73235730962155	2.85303044590630
O	-1.75168806112359	1.47873447471040	1.34326230770688
H	-2.25718885490289	1.88067426375214	0.61754806297323
H	-1.81290569278544	2.08366149878174	2.09650044866874
O	-1.76193876444394	-1.47139470191797	-1.34551139736157
H	-1.82418675146485	-2.06791291962184	-2.10541101500267
H	-2.24452680980401	-1.89499952990405	-0.61706762068891
O	1.76280720761700	-1.93337435938510	-0.40330953679063
H	2.25617796365568	-1.94185875582292	0.43285097217184
H	1.76917775703641	-2.84004415889762	-0.74251118997936

Pb(H₂O)₈²⁺

Pb	0.03795855961405	-0.01506062458605	-0.06724327259388
O	0.48290657318410	2.68278094390118	0.12427653742248
O	2.21423462176361	-1.69542044290220	-0.05566629752256
O	-2.65462058921306	-0.75566416102066	-0.15415092321962
H	1.02100950132228	2.76051553019023	-0.68443685446187
H	1.94978261112267	-2.27869083465198	-0.78765206774690
H	-2.81792154068025	-0.22050487298412	-0.95424755353164
H	0.00983674739682	3.51715791445052	0.24256028434362
H	3.18037247409095	-1.68047840201999	-0.03277410508995
H	-3.24432888156601	-1.52009350452145	-0.19618843646204
O	1.85274365618545	1.48254363472201	-1.89489339025820
O	0.05545105852071	-2.47446158621628	-1.51809872671438
O	-2.01935702975403	1.08441361373593	-2.05081304806229
H	1.73227963333751	1.63371130409560	-2.84379869419712
H	-0.10898778419214	-2.77633161163127	-2.42286306963267
H	-2.07238356896474	0.92126050815994	-3.00435255346576
H	2.81254605022744	1.41524920672463	-1.78241716646670
H	-0.39040352647581	-3.11974928743011	-0.94863044844309
H	-2.44022614955586	1.94938580991461	-1.93322854562649
O	1.65446423400747	0.83392899447300	1.61529430079652
O	0.01481907588518	-2.02592162083461	1.42078729408363
O	-1.55194370703825	0.76382273343440	1.68063544229338
H	1.55161278323466	1.79960215078730	1.55991106166435
H	0.94906592199220	-2.29691336614770	1.42972627183034
H	-2.39514162476931	0.33999934451037	1.44193991133887
H	2.15190993555133	0.61304465169260	2.41259418893941
H	-0.3393999909496	-2.12468183338864	2.31492815647046
H	-1.63628003613204	1.18655580754274	2.54436270431209

Fig. 3 & Fig. 4

-COO-

C	-6.32336778889846	0.64372105862141	0.00000853309395
C	-5.74291745886350	1.91662284799062	-0.00000540771931

C	-4.35207643039129	2.05057660317440	-0.00001934184769
C	-3.52342741007275	0.92334075338610	-0.00001755375372
C	-5.50193797316743	-0.48892174316953	0.00000157735303
C	-4.11207365467853	-0.34541657211621	-0.00001417264905
C	-1.97007330626235	1.07707816431505	0.00000331908433
O	-1.33624331592140	0.00248607374203	0.00001232993384
O	-1.55944991350357	2.25446176169288	0.00003132682502
H	-7.41417621146387	0.53467728024893	0.00002668667919
H	-6.38223658156422	2.80738228297378	-0.00000088793925
H	-3.85336287673586	3.02413010824880	-0.00002447607959
H	-5.95300436536510	-1.48815696804415	0.00001325739057
H	-3.42907271311163	-1.20002165106410	-0.00001519037132

-NHCSNHCH₃

H	1.52902053774405	-4.57566984890437	-0.73512617952077
C	0.56187402205409	-4.46052874863417	-0.23769493978749
H	1.17365815000380	-5.53436471544522	1.53917911270937
C	0.36347379260996	-5.00021676795598	1.03557800709334
C	-0.46241293393616	-3.77922830165584	-0.89282242766595
H	-5.06408005543694	-3.17786712816652	-2.48013390626597
C	-0.87580937502448	-4.85189036808429	1.65816713247746
H	-0.30814437449821	-3.35749184266633	-1.88527125574284
H	-1.04469526768184	-5.26707121434711	2.65544495002346
C	-1.90326403382336	-4.16033432076523	1.01496431797971
C	-1.70027155804703	-3.62026037387210	-0.25970265121480
C	-5.20498592679940	-2.17671289681133	-2.03578053366685
N	-2.79108084237629	-2.97238964976206	-0.89604051033274
H	-2.87100494651719	-4.02915696715056	1.50958570669141
H	-3.69856781477054	-3.34785451923665	-0.65065035925167
H	-5.60569373155370	-2.29624024018347	-1.01188912884728
H	-5.96880153500577	-1.65290484399059	-2.62529614609963
C	-2.77370853162367	-1.78482464491311	-1.57483984665805
N	-3.98421326327566	-1.40410241787776	-2.06395841448572
S	-1.43220311587109	-0.82731889665376	-1.81024220394838
H	-3.95886919617054	-0.52006129292349	-2.55547072348658

-SO₂

C	-6.14503551268153	1.02861660985501	-0.03454353100800
C	-5.33727546308097	1.87867850436538	0.72858346779217
C	-3.95319211789321	1.69823543052970	0.74995650664132
C	-3.37253843468936	0.66910919828324	0.00606067490876
C	-5.56061879515268	-0.00714832378801	-0.76838201571180
C	-4.17495192594668	-0.18670420666682	-0.74763154903446
S	-1.56868196096180	0.48117091365441	-0.01783874861796
H	-7.23131523165802	1.16947229780041	-0.05170174221189
H	-5.79299878147295	2.68569644871281	1.31282795372327
H	-3.29697903190226	2.33333252992915	1.35115291109097
H	-6.19075147493866	-0.68309284493229	-1.35688268909519
H	-3.68307036378369	-0.99609759531147	-1.29341515427986
O	-1.36512052211118	-0.93468059331430	-0.39303065975892
O	-1.16347525515297	0.82368419218881	1.36104748738132
O	-1.13278512857401	1.45604743869395	-1.03693291181973

-NH₂

C	0.12040253021069	-1.11124495435188	-2.85182263151053
C	-0.98398299456322	-1.53269993368585	-2.10789850345746
C	1.25351758748866	-0.65495296323993	-2.17445345227200
H	-1.88202040848209	-1.89368477409353	-2.61833519521012
H	2.13049880443624	-0.32085986867272	-2.73721709493894
C	-0.96122721644767	-1.50114499307758	-0.71481502573524
C	1.28678770758118	-0.61924645035310	-0.78157943731435
H	-1.83529218154439	-1.83154137061404	-0.14462231875708
H	2.18053679381852	-0.25695678192850	-0.26365672766673
C	0.17709972084425	-1.04198695395766	-0.02834655901639
H	0.09805552322938	-1.13842089677610	-3.94431595503790
N	0.18696862570404	-0.96351800813416	1.36112403783345
H	1.10235857569508	-0.95005650453342	1.79383937876735
H	-0.46087984242470	-1.57676398037750	1.84043875639796

-CONH₂

C	-4.55361483447483	1.75703171526908	-1.55723721652862
C	-3.37800455441053	2.13995684096656	-0.90629781610647
C	-2.83202504791836	1.32495101390124	0.08353014914576
C	-3.44672153051316	0.11382649490428	0.42059068578871
C	-5.18159810358580	0.55851561882326	-1.21355228001019

C	-4.63013867093324	-0.26151453916745	-0.22737530630597
C	-2.79899311507707	-0.70798939713984	1.50848427971725
N	-3.15650191785668	-2.02823030548276	1.55690405321861
O	-2.01228641464041	-0.21943362478386	2.29643787325380
H	-4.98560537372037	2.39867789660445	-2.33068437461056
H	-2.88834830828485	3.08190521395422	-1.16832705027711
H	-1.92255813032321	1.60709260333669	0.61892834972593
H	-6.11154251895825	0.26513463966364	-1.70825554498783
H	-5.14834231365128	-1.18239908399810	0.05452815434188
H	-2.66038996717752	-2.60610898616446	2.22435265430934
H	-3.58773919847438	-2.48199610068694	0.76454338932545

Non-functionalised UiO-66

C	0.00217858224471	0.07187304694680	-0.84047163889942
C	-1.15458156383712	-0.28238181115279	-0.14200390791182
C	1.15893955399898	0.42612684017406	-0.14200409906697
H	-2.06011477005164	-0.56121296895870	-0.68871552210539
H	2.06447291236505	0.70495626154790	-0.68871600265512
C	-1.15457943037990	-0.28238662085986	1.25496868509535
C	1.15893794197352	0.42613091136484	1.25496872701485
H	-2.06010758793298	-0.56122971997851	1.80168303670517
H	2.06446591122174	0.70497391236324	1.80168340928899
C	0.00217906589289	0.07187256174082	1.95343719144278
H	0.00217774027021	0.07187152818983	3.04757988421911
H	0.00217840623452	0.07187154662235	-1.93461436312747

-SH

C	-3.81874921477710	1.42025877090554	0.00000113327444
C	-2.42461196182777	1.47763138769871	-0.00000555938740
C	-4.47740705824593	0.19003454925602	0.00000220960873
C	-1.67331832020669	0.29579639532065	-0.00000728104218
C	-3.72743906701162	-0.98797791761392	0.00000375176765
C	-2.33408229407642	-0.94011708118305	0.00000171315257
S	0.09765703767740	0.28171628894922	-0.00003450097500
H	-4.39315305851444	2.35095245481323	0.00000034566671
H	-1.92103609124142	2.44839029736925	-0.00001516596666
H	-5.57009915877072	0.14921609757226	0.00000103482431
H	-4.23128924664037	-1.95863254470994	0.00000468020972
H	-1.75287677344632	-1.86676392979397	0.00000195181625
H	0.26727520708143	1.61574523141602	0.00004568678086

-SO₃H

C	-6.45689416198141	1.32337686280000	0.04893206941734
C	-5.81524607340624	1.57181558291076	-1.16745264678815
C	-4.47140292289223	1.23628344704311	-1.32897923890975
C	-3.79129512478072	0.66089972070584	-0.25550275275318
C	-5.76341881059184	0.73256262905683	1.10868687676376
C	-4.41794144740949	0.39528954937756	0.96153643354749
S	-2.07434399394177	0.27084581882676	-0.43739378739597
H	-7.51127283680819	1.58734441249517	0.16889807415051
H	-6.36594756257259	2.02264287196838	-1.99718247778539
H	-3.95114904673955	1.40048370450345	-2.27551490681394
H	-6.27323651835928	0.52914884638273	2.05416008993168
H	-3.85264351701022	-0.07731135151888	1.76794951637123
O	-1.76865007355706	0.13214114939937	-1.85144948445601
O	-1.72139906427126	-0.73276189774447	0.53866698344565
O	-1.36999429551456	1.65109595137689	0.05360709867865
H	-1.07760455016353	2.12700270241649	-0.73944184740393

-NCS

C	0.15512133076545	-0.95137278651378	-2.87193649297693
C	-1.04408975978175	-1.42286960885544	-2.33174346228945
C	1.24600351270316	-0.70666210246047	-2.03453631978224
H	-1.89980045438605	-1.62018809130959	-2.98323896025544
H	2.18668568778122	-0.33903438761812	-2.45327707373804
C	-1.15988169104880	-1.64777426920937	-0.96118554645581
C	1.14534163578728	-0.92686804519544	-0.66189850918835
H	-2.09106180405840	-2.01603785525811	-0.52488081883627
H	1.98887249947921	-0.73702457417990	0.00549710823428
C	-0.06215278219850	-1.39616776246446	-0.12575516139967
H	0.24090471500648	-0.77579467387040	-3.94765219870806
N	-0.17161247232319	-1.61018561325126	1.23525439506887
C	-0.34768527794912	-1.78853107790680	2.39127033100267
S	-0.56867913977701	-2.02857315190682	3.94204170932446

-BCOOH

C	-6.27801636808523	0.66558772181979	-0.00005372646023
C	-5.62322042819125	1.90009391880908	-0.00003104355519
C	-4.23051891686811	1.94730394663527	0.00005188504969
C	-3.49064665270516	0.75882732851908	0.00011556167900
C	-5.54108707281749	-0.52112654889970	0.00000669579114
C	-4.14700921666170	-0.47792119909737	0.00008649222982
C	-1.99955306286980	0.86305626128434	0.00022763635918
O	-1.38556756119352	-0.33508294709732	-0.00009805599217
O	-1.38440683145922	1.90101427207954	-0.00004179816440
H	-7.37165430936993	0.62809814343909	-0.00012074104954
H	-6.20130428013413	2.82807928719600	-0.00007638803085
H	-3.69244193452050	2.89813666558541	0.00007804232457
H	-6.05610516427039	-1.48556605897265	-0.0000988055283
H	-3.56076663829142	-1.39883728302822	0.00013609501242
H	-0.43367156256213	-0.15065350827232	-0.00027077464061

-NCO

H	-1.57712733418277	4.13703397269153	3.34356607691602
C	-2.00906413759556	3.13550277136659	3.42086023266096
C	-2.51591179925751	2.68314030273253	4.64139091919946
H	-2.48613740908022	3.32964170297473	5.52250624085782
C	-3.05947729616991	1.39995007055139	4.72977947458975
H	-3.45759644057566	1.03807080485877	5.68163543255114
C	-3.10078551172794	0.57164859667692	3.60875930271296
H	-3.52396009728662	-0.43354902848860	3.66183735780978
C	-2.59695958678761	1.03040631089455	2.38652379325376
N	-2.65663633071377	0.18299370966993	1.27542700994248
C	-2.04611723540169	2.31614544093213	2.29339158459411
H	-1.64884265666517	2.66661520484215	1.33698470356944
C	-2.42183842392065	0.12546919004840	0.09663584790241
O	-2.22497574063491	-0.03971904975103	-1.04438797656009

-COO-Pb(H₂O)₄²⁺

C	-5.83554926769442	0.27846624149331	-0.20879037713859
C	-5.08902732325202	1.06833846904421	0.67064900612569
C	-3.76633434726236	1.38314405181010	0.36817525370616
C	-3.18828016757872	0.90122832456169	-0.81532765346166
C	-5.26202402408035	-0.20342366808988	-1.38876791905000
C	-3.93809092979861	0.10458751017909	-1.69263371718132
C	-1.78276301746001	1.24023385597871	-1.14749997200209
O	-1.23147307414306	0.78776054441969	-2.19887667038073
O	-1.10533021709239	1.99881463064008	-0.37961499911719
H	-6.87499974480712	0.03599802353156	0.02856845672146
H	-5.54311177940752	1.43763510616879	1.59355217990141
H	-3.16865005729100	1.99992574513586	1.04289692635115
H	-5.85098115367793	-0.81984270465902	-2.07284079667648
H	-3.47225264743688	-0.26459522370172	-2.60879712337141
O	-0.37117871375286	4.08624191539719	-2.29394220761859
H	-1.17960490791630	4.28084764491850	-1.80022429682644
H	-0.63919204300294	3.84441946296538	-3.20014983420184
Pb	0.84576547459961	2.01508543638632	-1.66484737587423
H	0.00364564501889	2.07639517382186	-5.15857216324675
H	0.28916807721537	2.90666676824225	1.08496121544442
O	-0.25785353417273	2.23062752239196	-4.24168071106172
O	1.16387454118531	2.93907766925138	0.66981084511812
H	1.68890897108590	3.60218954479515	1.13538334483401
H	0.12686726187411	-0.88707722702342	-1.22528257992942
H	1.34557191383218	-0.99064294310069	-0.25900045327950
O	0.94432131316079	-0.44759275003957	-0.94969145582493
H	-0.88732624814446	1.52860087548085	-3.99875692195925

-NHCSNHCH₃-Pb(H₂O)₄²⁺

H	0.79774914717813	-5.83661638974743	-1.56939851072166
C	0.08077585628560	-5.40211930805016	-0.86759857467703
H	0.98619355622815	-6.32309561807160	0.86852972333387
C	0.18344296846180	-5.67747761315899	0.50214747491841
C	-0.96198168219573	-4.60355877450438	-1.34778190295523
H	-5.13961632840716	-2.94557412925689	-2.77937493597597
H	-0.74822828502775	-5.14328173805098	1.39724008140484
H	-1.07005943567584	-4.40504762843571	-2.41757147906478
H	-0.67741139741921	-5.36693382334227	2.46507423887853
C	-1.79110428383385	-4.33254921959612	0.92672881286544
C	-1.89484437519346	-4.07053451151787	-0.44670657556311

C	-5.26387863551296	-2.09428664775530	-2.09078911817779
N	-2.98530482977910	-3.28287605702692	-0.93631504333070
H	-3.88394518504395	-3.75430159199019	-1.01198409096735
H	-5.72193255049063	-2.43420178035282	-1.14738882355869
H	-5.94523209919751	-1.37291929606944	-2.55771038722846
C	-2.90911942943855	-1.99987134574804	-1.32484282746933
Pb	0.41393698999297	-2.24002038237495	0.30685633047627
N	-3.98560700440170	-1.42831895858026	-1.84676682632498
S	-1.47843406743183	-1.03444121770335	-1.18518249613340
H	-3.89094482509402	-0.44977785784396	-2.10296161900165
H	-2.52892372663651	-3.91549394987254	1.61714285916491
O	-0.70420367721218	-1.18794511691367	2.20862554874683
H	0.02744098509658	-0.96205335179903	2.81425514780371
H	-1.41466991787398	-0.54010043997175	2.30698370453134
O	1.74947462499404	-1.59262693206817	-2.01703003103646
H	2.59258517371988	-1.91538821355309	-2.36985947605754
H	1.17325947503325	-1.47810494879103	-2.78875670488717
O	1.30587075920565	0.09941961267882	0.08772689962703
H	0.80016842548647	0.92320066101040	0.14573889050107
H	1.71813052375279	0.08572010820455	-0.79382988470119
O	1.92877150774103	-1.32245375481654	2.61150726040021
H	2.43168779416819	-1.76515216380217	3.31115496867295
H	2.46492394852149	-0.55763762112783	2.35360736650711

-SO₃⁻- Pb(H₂O)₆²⁺

C	-5.86476077160988	1.45338720758690	0.45608632513354
C	-4.83032217211949	1.98808269898667	1.23206396131316
C	-3.50504724143209	1.68500348206029	0.93162509305551
C	-3.24454734854562	0.85110511004180	-0.15966338280892
C	-5.58400361415188	0.61228771629365	-0.62250420391248
C	-4.26104078095698	0.30295154916808	-0.94132702824093
S	-1.57187916947693	0.48544780091654	-0.54661278361091
H	-6.90317724609719	1.69078094768098	0.70194377661317
H	-5.06136038352756	2.63484440816708	2.08214256573874
H	-2.68522861852793	2.07591065156344	1.53894049264186
H	-6.39734481484428	0.18771581410703	-1.21595849051408
H	-4.01446717700231	-0.36291033671752	-1.77096091334740
O	-1.54943277261310	-0.54349075520949	-1.62097941082041
O	-0.84143228896660	0.12090708273499	0.67695978291635
O	-0.98852605306162	1.79366537092086	-1.11246961074963
H	-1.04836552209556	0.27440108729396	-3.21404805176526
H	1.54549028444970	-0.99739200610313	-0.77129622288996
O	-0.43656543903404	0.82845406561216	-3.74284005946933
O	1.17007530664946	-0.66888269740034	-1.60087413019982
H	-0.15336189902201	0.27948632140252	-4.48579376416938
H	0.24896827293234	-1.00495690918261	-1.62571025856271
Pb	1.15632681598371	1.82392166275528	-1.96872818975191
O	-0.53918736734798	3.98013514253512	-2.48355037574527
H	-0.82501403817179	4.33042655142030	-3.33744604177915
O	1.51826909466952	1.41785195932058	0.44640632321311
H	1.46298439776211	2.30636097577353	0.83173077604324
H	-1.27511414396858	3.44038883270505	-2.14434539485363
H	0.72229730912567	0.93512195801213	0.77267865234313
H	2.01838187848966	4.75182874135479	-0.47888759849586
O	1.30744385244284	4.09707347693507	-0.48445832897121
H	0.57193165006851	4.50922208926420	-0.97370350835352

-NH₂- Pb(H₂O)₆²⁺

H	2.64158239032298	0.40022404616755	0.97736947165231
C	1.73060991047498	0.24739334185104	0.39335371985075
C	0.48003030994977	0.30227610219144	1.01492327642069
H	0.40808748128192	0.49977400784645	2.08799104063082
C	-0.68479972836509	0.08359098436168	0.27301013549481
H	-1.66014821339792	0.09054062536767	0.77362837541259
C	-0.59543837725233	-0.20501121727084	-1.09739943093777
N	-1.80562259456037	-0.29089599271975	-1.86521926752313
H	-2.50556290535682	-0.88308853745477	-1.41242349330007
H	-1.63924661098427	-0.66579845923100	-2.79959926783073
C	0.65470066717098	-0.26577012576626	-1.72264482354306
H	0.72588534313526	-0.50219872325947	-2.78805479612441
C	1.81324459819870	-0.04504536467548	-0.97356142087703
H	2.79059231460445	-0.11771431899187	-1.45865724119355
H	-5.10010449541028	4.10127950296392	-0.83493923186813
O	-4.14975395685530	4.20497400398490	-0.67049211907971
H	-4.10752003250330	4.64125388811548	0.19491799095226

H	-3.85620663779672	3.10297649304935	-3.94716764637492
O	-3.74282395350162	2.23488943019131	-3.53003494826758
H	-4.35835463362821	1.61857685232437	-3.95295931004331
H	-3.16141247913269	4.98669142536938	-2.14306215514063
O	-2.52528454927194	4.60540339016813	-2.77839784550653
Pb	-2.09989560009205	2.32680666012979	-1.64505562841219
H	-2.04861633694773	5.33551816283057	-3.19814145073111
O	-0.62166107577290	2.09412515688540	-3.55803349968702
H	-0.75666715739223	2.13365341266160	-4.51551276543301
O	0.45608968867772	3.01219624574859	-1.22435144260287
H	0.83244123521988	3.86833513150310	-0.97057381385372
H	0.26207347291756	2.43584354727026	-3.34343345295346
H	0.99051192626771	2.34991032838717	-0.74895895913004

CONH₂- Pb(H₂O)₂²⁺

C	-4.77490203097604	-0.10200020791856	1.30587200649004
C	-4.58621328443540	1.26698985590910	1.50876226911752
C	-3.82969346865672	2.00925186456960	0.60147272666423
C	-3.25353670167131	1.37492739298600	-0.50889117134020
C	-4.20203430417040	-0.73859793772015	0.19848681961959
C	-3.43510339528887	-0.00523954116877	-0.70604099190217
C	-2.41162520538344	2.13067788402764	-1.46525811462466
O	-1.41831780547881	1.55850312500778	-2.01974124333370
N	-2.69396510670395	3.39179796311529	-1.73425772740781
H	-5.37736678242074	-0.67832048464457	2.01334045239280
H	-5.02955176529737	1.75939262322413	2.37799535015908
H	-3.66685778221298	3.07591622085112	0.78253872179076
H	-4.37400716125474	-1.80544931312606	0.03272279629075
H	-3.01323990516808	-0.48791228375108	-1.59202102526220
O	0.21480349882381	4.03231140034146	-2.23158408403404
H	0.55086906317363	4.88634588040503	-1.92120606340804
H	0.57373248918122	3.90847386911127	-3.13041558988350
Pb	0.73821209449214	1.61776996970236	-1.40689108799685
H	2.41248354772088	2.55152267241772	-4.27789951597535
H	-1.25131384415767	-0.28067366598780	0.23389634297540
O	1.53603380430265	2.35030008917281	-3.91559764761476
O	-0.32636844945138	-0.01285995176930	0.37310870065842
H	0.08063172190715	-0.71616447510499	0.90082081080658
H	-0.62865925707785	-0.28516679347948	-3.43484275755443
H	0.73413748451378	-1.02583428838698	-3.47178776364320
O	0.31952171738805	-0.17414311725907	-3.26869320084280
H	1.17910446152070	1.64049443856917	-4.47293674235638
H	-3.54542529265954	3.82838939743763	-1.39677337285497
H	-2.04234834862042	3.92840569683239	-2.30329120047836
H	-0.53934468208187	2.04071654486423	1.25274658509979
O	-0.33882376777211	2.74588225007756	0.61735611679055
H	-0.15364154208401	3.54427292169421	1.13143960165816

Non-functionalised UiO-66-Pb(H₂O)₆²⁺

O	-0.24979673047064	2.17115680905577	-3.52696447782368
H	-0.45674679496152	2.78237260841526	-4.24917045371165
H	0.02235997531374	2.72153989040783	-2.77720087860506
Pb	-1.13802684021055	-0.17792886011667	-2.85473888294071
H	1.76610610627085	0.47443881351832	-3.66237768337277
O	1.35889812881953	-0.27738402831973	-3.20661150194908
H	1.96545173198890	-1.02622921011749	-3.30149409156405
H	-0.90084821216520	-3.14998776582079	-1.57227745855537
O	-0.63582017931220	-2.23884455014786	-1.37777977094517
H	-0.22354576032670	-2.27247062571418	-0.50206517931469
H	-3.52094650582555	1.47779115527500	-1.18887586701661
O	-2.94700363187295	0.71181437723357	-1.03407300570954
H	-3.47453683677639	0.12590446184190	-0.46954154942290
H	0.75931637043897	0.92606033400540	-0.45312999716962
O	-0.11909196985321	0.98230860124590	-0.85593620941455
H	-0.74800886965868	1.21352600646232	-0.15504427260329
C	-1.36915251933122	-0.76462872338744	-5.85512133078190
C	-2.47993640464503	0.06632144751371	-5.64172990827663
C	-1.33527330624329	-2.04825666339710	-5.28764063718198
H	-2.52575504370164	1.05083715355841	-6.11605879123307
H	-0.48768308427766	-2.71114028858846	-5.48497742751877
C	-3.55359427748735	-0.38291550320198	-4.85835806100435
C	-2.41257657222670	-2.49828777991067	-4.50788180533162
H	-4.43181254363655	0.25390676327999	-4.71829268607184
H	-2.40872137345215	-3.51479075678350	-4.10347771951283
C	-3.51977087497981	-1.66514113360100	-4.29101592136900

H -4.37230004308220 -2.02800148259593 -3.70975811661923
H -0.54624793833460 -0.42747005011052 -6.49208702767945

-SH-Pb(H₂O)₆²⁺

O 0.37536380677426 1.81245227953501 -1.66334530286248
H 0.20698446201657 2.69203018042075 -2.03042153575469
H 1.20539876781514 1.84953605263006 -1.15068934202817
Pb 0.42660578364861 -0.50777655466768 -2.53478253745404
H -2.18460993132934 -0.97775093125509 -0.44254197190020
O -1.71607437057344 -0.29238289013464 -0.94365943294180
H -1.72649785244623 0.49480372940956 -0.37742985792898
H -1.81698596318828 0.94234081851143 -4.37571622818692
O -1.63767565928586 0.28193845653431 -3.69067499040179
H -2.36898588487457 0.32037844636309 -3.05269600924305
H -1.17291053896519 -2.06299242734593 -4.78315988488097
O -0.34646162593262 -2.27211561210322 -4.32299511533841
H -0.23281973775646 -3.23035171375288 -4.41001823100840
H 3.34690430678045 0.39167149110773 -1.18537775454105
O 2.46391224929903 0.38058858504446 -0.77652419617049
H 2.61452031329239 0.11097995612561 0.14235584398544
H 4.52772529759959 -2.98241915058775 -3.00525278271601
H 2.57123066628775 -2.11683982213644 -4.27797756495433
C 4.39719126345386 -1.90445300839809 -3.13382092341395
C 3.29359397512546 -1.41861199087255 -3.84114213355750
C 5.34062077259643 -1.01594506210581 -2.61125836413817
H 6.20876393701073 -1.39914248878530 -2.06852985187785
C 3.15227413705213 -0.03594909997570 -4.02941818360089
S 1.70186573108301 0.65016969063146 -4.82560602350312
C 5.19396803525490 0.36180349215087 -2.81040963686045
C 4.09962239463669 0.86099776600919 -3.52583020438592
H 5.95131669069419 1.05389344886613 -2.43148060015717
H 4.00048760462112 1.93497264313823 -3.70801689240451
H 1.45022136930938 -0.36257628435680 -5.68178029177367

-SO₃H-Pb(H₂O)₆²⁺

C -6.33406702286076 0.12157859309248 0.51933302026826
C -5.49897275345354 0.54208852675804 1.55955218074171
C -4.13674938878963 0.71869657933348 1.33218764553313
C -3.64822218253747 0.46660896612887 0.04344009350898
C -5.82367482004731 -0.12193957279484 -0.76120714621118
C -4.46532432896308 0.04854643409746 -1.01509826018254
S -1.93488511886164 0.62311783093696 -0.20345586300542
H -7.40209034297054 -0.01678911266019 0.70828566473215
H -5.91013457563717 0.73481895673520 2.55335980258057
H -3.46741189674113 1.05073302572457 2.12944706514981
H -6.48964406371386 -0.44370296695923 -1.56533705340729
H -4.05313309991934 -0.13081941130402 -2.01100583110427
O -1.31795412017443 -0.82173950441003 0.17930333438145
O -1.32506782164685 1.53773197287670 0.74948736583109
O -1.61719299908412 0.85304315935902 -1.63019589238066
H -1.96226272786631 2.54974449124625 -3.13834821363997
H 2.08634801955389 0.16563468864707 0.00054836184097
O -1.16611930950028 2.84339968283173 -3.60821727693658
O 1.25784104971746 0.09769628672124 -0.49335813274025
H -1.39982725805919 2.81129652966506 -4.54807436170977
H 0.69128329478358 -0.54977120946486 -0.04394004684202
Pb 0.86000231481592 1.59826099756014 -2.45857081133488
O 1.34355458346770 4.05385850418631 -3.05795799236829
H 2.15428247965598 4.50923611399302 -3.32782237455213
O 0.52026367096854 2.96075365408693 -0.58527748603891
H 0.38786141717280 3.91233073739156 -0.70369590338267
H 0.61529366158658 4.47547699249819 -3.53890309651206
H -0.10365069040233 2.61981734898712 0.09721497922056
H 3.40482806961773 2.68120674453752 -0.85165442310178
O 3.23292231641901 1.99761151369113 -1.51582834880181
H 4.09978795600342 1.72558642255039 -1.85246427790839
H -1.86004431253311 -1.55716297604377 -0.16170672162744

-NCS-Pb(H₂O)₆²⁺

H -0.66971182440449 2.82698603415711 4.92674816054302
C -1.46343591401311 2.38687854968758 4.31834857728042
C -2.80095781580536 2.52489956760214 4.70296172075194
H -3.04879461707725 3.07561982866572 5.61396121959246
C -3.82344271671390 1.95764458417114 3.93689183639866
H -4.86576449622807 2.06196917158003 4.24779342833850

C	-3.51934341136699	1.25114607727670	2.77584067196432
H	-4.30533015770361	0.79385456796528	2.17063470702905
C	-2.17471679994890	1.12475055653963	2.40498196697679
N	-1.86171535738770	0.41495402620588	1.24191015423475
C	-1.13664417687191	1.67909655450738	3.16434263352149
H	-0.09561071319517	1.54685427249486	2.85996860928812
C	-1.63227153412935	-0.16319365754062	0.26176615303765
S	-1.35616010513479	-1.03548192744724	-1.10284355490596
O	1.63472049967711	-1.71095519149837	-2.7272070999536
H	1.55758243452329	-2.33345264228432	-1.98700354228408
H	2.55066311240526	-1.80397788831429	-3.03272642854796
Pb	0.12317260916651	0.67394765687204	-2.68011994551068
H	-0.26687264769879	3.10492616773658	-0.43634468851161
O	-0.71836758975802	2.48128524112920	-1.02372932222013
H	-1.53829884309019	2.91686332509207	-1.30032905561602
H	-2.94003183796261	1.04471690834493	-3.28016087234051
O	-2.07973242241291	1.48022678684216	-3.36941968913321
H	-1.97193935588573	1.76528487441321	-4.29509271971184
H	0.15803363761096	-1.80816548514298	-4.08443302738229
O	-0.51428503168040	-1.12798354744690	-4.27746946456857
H	-1.34174759137390	-1.59012797988774	-4.47487009960308
H	0.22700090701993	2.51763211611320	-5.63320483917475
O	-0.14835783423736	1.71726059796517	-5.23472892596906
H	-0.07852240632226	1.03444185420030	-5.91986156348203

-COOH-Pb(H₂O)₂²⁺

C	-6.39428416174392	0.68013044511605	-0.07085470137548
C	-5.77807488562282	1.65227002243793	-0.86539374857347
C	-4.39240390257944	1.67496100422012	-0.98086283930401
C	-3.61741623019585	0.71086655161752	-0.31255706313392
C	-5.62927728889962	-0.27044968670151	0.61334739422048
C	-4.24402824547363	-0.25923051850757	0.49352861524102
C	-2.15888147697554	0.75497054308587	-0.47377935711782
O	-1.43506285101448	-0.31736588727241	-0.13841475077747
O	-1.55350183127185	1.73650583872278	-0.91175268136885
H	-7.48405934233429	0.66455813612053	0.02068712821314
H	-6.38448334684638	2.39156731528214	-1.39424565993953
H	-3.89803817313801	2.42692265141496	-1.59997738308818
H	-6.11616217077407	-1.01680122755678	1.24546493468653
H	-3.67097508359068	-0.99463668974486	1.07009358813397
O	-0.58650036415161	2.89981237305415	-3.54753142849400
H	-1.45157653896665	2.73286835721655	-3.94356366736884
H	-0.24485399804554	3.75794597887542	-3.85474727931411
H	1.74449884874617	1.03813654474356	1.30279857633107
H	-1.35960972918532	4.05625268445610	-0.12852697661669
Pb	0.69026187553153	2.32663727668192	-1.55085055255144
O	-0.44346773034096	4.25625803980087	-0.37271268628246
H	-0.10154669453184	4.84968173997282	0.31229648565781
H	1.08299594304861	5.58607470282136	-2.65318088577702
O	1.32024353279276	4.72012654669063	-3.01726999895121
H	0.12364667460019	-0.76835405022360	-1.99386598971028
H	0.72349320745951	-0.37272039160546	-3.37000639833466
O	0.39010494475625	-0.01252237041370	-2.53550968825942
O	0.98566460941267	1.08189304581862	0.70358802255311
H	0.39450605337441	0.35635808917567	0.95057255700359
H	-2.00829931647809	-1.05542762482604	0.12773426592615
H	2.11039767243916	4.88946055952578	-3.55299783162762

-NCO-Pb(H₂O)₂²⁺

H	-2.63103195759139	3.82404305920828	5.40601645086364
C	-2.75117200238994	2.91929055010153	4.80518963152363
C	-3.45711766448958	1.82685500733840	5.31511159389108
H	-3.88964391389945	1.87693412098695	6.31721037397139
C	-3.61676887065740	0.67049539572403	4.54740280161354
H	-4.17330677961836	-0.18114292990406	4.94605246401102
C	-3.06804892993248	0.59631648366176	3.26833928180512
H	-3.18676912410342	-0.30100022926362	2.65664947255207
C	-2.36130914865939	1.69716230684038	2.77630765724880
N	-1.79886964040345	1.62750350574722	1.48931958679316
C	-2.19495165941227	2.86312478582962	3.52846422775405
H	-1.64049725265316	3.70988139179011	3.11792347879412
C	-1.33161233186086	1.58147194157949	0.42349819555524
O	-0.83958301455365	1.53405652967011	-0.68223896456841
Pb	-0.12474448835186	0.10738872230449	-2.74897424337372
H	-0.06295254843633	3.04925704180805	-3.90746414942143

O	-0.45453140257621	2.45178151895589	-3.25423556891216
H	-0.76461852331159	2.98238929039466	-2.50319472319966
H	-2.01146635556818	-0.93228017504140	-5.31150119549977
O	-1.57632749063431	-0.11777957213300	-5.01505670898644
H	2.12103541962133	0.49668588452733	-4.95951774418434
O	1.19246737490095	0.28697707433625	-4.78449655436305
H	0.74183010291109	0.13033811416148	-5.62849665372597
H	-2.15597733845104	0.59391723304170	-5.32718409643976
O	1.69737532414437	-1.81238431243409	-1.87158112306155
H	1.52062576113332	-2.35833255709320	-1.08952740461975
H	2.21464220515351	-2.39167437082788	-2.45297222854219
O	2.06497124832489	0.87967946541153	-2.01112202959104
H	2.51101972822045	0.11239416255694	-1.61258960793815
H	2.31359327314480	1.66843056072079	-1.50761221994903

Fig. 5

-SO₃⁻-Pb(H₂O)₆²⁺

C	-6.08495174673380	0.83795539621928	-0.34077804026482
C	-5.43239478547073	2.03386890706770	-0.01769593785820
C	-4.07126244291878	2.02953501620713	0.27326271765844
C	-3.39128248427067	0.80823580002494	0.23493298007899
C	-5.38591432173382	-0.36980517887304	-0.37195997138967
C	-4.02123493429475	-0.39485015048689	-0.07971720359903
S	-1.67849270650008	0.78706385074199	0.60528703956593
H	-7.15433902772636	0.85030339213486	-0.56819367182347
H	-5.99197402635035	2.97215153870989	0.00993120364652
H	-3.54060916595467	2.94880949056113	0.53400587738743
H	-5.90325785086533	-1.29931443126779	-0.62144230218687
H	-3.44894245503773	-1.32489322447782	-0.08854842168014
O	-1.19035851611190	-0.58942563211356	0.63131932500817
O	-1.47983676945264	1.50856195477975	1.93448995174001
O	-0.94538992404940	1.67760297741477	-0.37879801965686
Pb	0.35946689469329	2.81300405268811	1.35935539316776
O	1.21682168794891	0.42170316422514	1.63390866684599
H	0.52594873110010	-0.23435228869730	1.40214370809019
H	2.05438740635060	0.05041996773186	1.32746352810997
O	-1.51300442978155	4.44362150554460	1.08073703304765
H	-1.76190758532790	5.18729460348543	1.64414684625192
H	-1.30745347347421	4.77869201446180	0.18651114051683
O	-0.34484787859626	3.05815866553477	3.77327662214763
H	0.16918351331148	3.00000038599427	4.58960452222094
H	-1.04766853022213	2.39094108498638	3.83635044549036
O	-0.15592811090514	4.09969334352847	-1.15904454173597
H	-0.56527404919076	3.26822298850293	-1.45781146974184
H	0.30318698156489	4.47786080537094	-1.91974742103794

-NH₂-Pb(H₂O)₆²⁺

H	2.66137246541033	0.32714706473714	0.98023528810143
C	1.74931605361377	0.19804983367983	0.39187016946058
C	0.49768632529745	0.28061927274314	1.00903253841261
H	0.42570021051230	0.47462482200815	2.08274174898173
C	-0.66905112854867	0.09527198796777	0.25944278701366
H	-1.64608997093102	0.12486908810084	0.75638337956017
O	-0.57631740286191	-0.18490718623017	-1.11141302018119
N	-1.78751645923900	-0.22607015929239	-1.89171287371189
H	-2.51176754568299	-0.79033415530627	-1.43943096463063
H	-1.63004996476181	-0.61897035572499	-2.82075634752181
C	0.67303872890109	-0.27436586141050	-1.73319873866675
H	0.74439642591965	-0.51293319952358	-2.79875869796322
C	1.83283313026934	-0.08875673672040	-0.97642845952851
H	2.81065124823237	-0.18276237255940	-1.45667804981500
H	-4.04103340829882	2.98414542786760	-3.87149266872379
O	-3.68193835454400	2.13357617575595	-3.57398005854716
H	-4.30459668343935	1.45138064180051	-3.86747439686597
H	-3.04871538179451	5.39395249853030	-2.24294017914521
O	-2.58030644358880	4.68091405513717	-2.70537366488825
Pb	-2.08785167045700	2.31809987855637	-1.65647448815148
H	-2.07277678502625	5.12697313021388	-3.40044055756243
O	-0.65345913180338	2.29092374831673	-3.54194087273948
H	-0.75527257635030	2.09219042714585	-4.48406269676094
O	0.42534902590374	2.99180210895509	-1.17937513069696
H	0.74414349422748	3.83694769214477	-0.82685299733017
H	0.26825978853723	2.52367034699170	-3.34196205361044
H	0.93809601050309	2.30714182611485	-0.71190899448881

-CONH₂-Pb(H₂O)₂²⁺

C	-5.54204723711706	-0.31224226614858	0.08069717123629
C	-5.17096026322181	0.75955355021771	0.89852370924159
C	-4.06930414622279	1.54072976047354	0.56263650476602
C	-3.32512139694900	1.24242267871425	-0.59314613543140
C	-4.80548308839690	-0.61511841475909	-1.06865429709992
C	-3.69495732087726	0.15432191694612	-1.40234343952697
C	-2.15295618981128	2.04643928096869	-0.98246879796889
O	-1.28247234282358	1.55861601429261	-1.77147706948597
N	-1.99767917919457	3.28079122589415	-0.50106131145768
H	-6.41389193155093	-0.91786043237346	0.34219627192823
H	-5.74160593726261	0.98265441572671	1.80305576199330
H	-3.78152017832287	2.35854747414428	1.22991093008558
H	-5.10502420169735	-1.44992696136317	-1.70687331866073
H	-3.12524397114837	-0.06360050480599	-2.30856286326670
O	0.34577966097065	4.26017299048695	-2.09790280514971
H	0.96733104986857	4.90254769305102	-1.71845796019280
H	0.04428937701695	4.66156658721781	-2.92895454151209
Pb	0.93521191643643	1.66586504994074	-2.08185449550936
H	0.29161092103523	1.58645097293334	-5.22815053746703
H	0.03345195581984	2.40251706605986	0.93964091322193
O	-0.10391799867395	1.71933474018812	-4.35301384372816
O	0.82128940426108	2.22386837167101	0.40548942965499
H	1.54219732101636	2.07781276337049	1.03724939982168
H	-0.46350730717530	-1.01898669922824	-1.48495564141762
H	0.99282672000329	-1.52732356475020	-1.71148463052319
O	0.43675555380495	-0.73356987943545	-1.70153890290573
H	-1.04473300475480	1.50457710623368	-4.44009672775266
H	-2.75741647344878	3.73562054542184	-0.00504469859866
H	-1.24850171158373	3.86062851891099	-0.88060807429410

-SH-Pb(H₂O)₂²⁺

O	0.53891157511936	1.17987757484641	-1.93586026236304
H	0.21014174630861	1.98921055044823	-2.35569754474870
H	1.31959870041650	1.38520980376685	-1.39386401375446
Pb	0.55115342188060	-1.07101724719916	-2.69217182739317
H	3.36155524276091	-0.39086442378559	-1.31282602263051
O	2.45762462541958	-0.41965337779607	-0.94999326052456
H	2.55385586823803	-0.77486068467868	-0.05264341876574
H	-1.97599711374468	-0.06819025411888	-4.43115702676930
O	-1.63306027414541	-0.25077769382386	-3.54347107448646
H	-2.39912488460467	-0.36020689368271	-2.95955159125539
H	-1.35212421509127	-0.26301809705157	-0.23156822203551
O	-1.22223511431464	-1.03117350760099	-0.80897817062763
H	-1.60205604427205	-1.78503534103686	-0.33032339753781
H	4.93543105449846	-2.94133291026568	-3.27143236708784
H	2.90962340328789	-2.36139043700755	-4.58219054959314
C	4.62909123161003	-1.89544270272758	-3.35938626919964
C	3.48371973997125	-1.56840641222959	-4.09016163501347
C	5.39053786046918	-0.88613095414602	-2.76033598042241
H	6.29371304666629	-1.14398881754558	-2.20050031964153
C	3.11599447272929	-0.22028703900007	-4.22835078418088
S	1.60250425005653	0.25555222797931	-5.06248944372189
C	5.01779364183614	0.45572525402280	-2.90584030962057
C	3.87930637475261	0.79658679539810	-3.64521534689299
H	5.63182448403322	1.24566289418258	-2.46419231394046
H	3.60865741535389	1.84648815919484	-3.79044980527174
H	1.58328949076414	-0.70251646614266	-6.01407904252087

Non-functionalised UiO-66-Pb(H₂O)₂²⁺

O	0.04291094355669	3.15590932533388	-2.78146645481835
H	-0.06620287496783	3.87551185873308	-3.42246304982425
H	0.40671333818893	3.57614053477321	-1.98729988670520
Pb	0.17376951161848	0.62573584073086	-3.33214250936113
H	-2.37966462548000	1.91246006240913	-1.96940801211481
O	-1.93960073113762	1.04890298400110	-1.99676428589517
H	-2.63394758758411	0.38284088957554	-1.87717176098037
H	-1.29968229831556	-2.28212514898738	-3.25967741093307
O	-0.83318732712346	-1.67642671251501	-2.66265526210527
H	-0.54894539743791	-2.22679009838889	-1.91704600941441
H	1.45697290152344	0.45554502177299	-0.38267171557903
O	0.67496729008218	0.59318519093734	-0.93822018775581
H	-0.08552005009177	0.73492858715589	-0.35263671796384
H	1.70725715485169	1.90550070043995	-6.57093646366975
H	3.00487700592382	2.64484307904933	-4.56682229375225

C	1.99521567295737	1.17886919035571	-5.80558799766695
C	2.72294600666993	1.59422677064894	-4.68029320128323
C	1.67099285853934	-0.17732221127110	-5.97184894244907
H	1.13024750146099	-0.50245872442242	-6.86550071097282
C	3.11908383723759	0.65402069941875	-3.71306332042691
H	3.72353689038564	0.97288656573758	-2.85820371029426
C	2.07242414332073	-1.11907800299292	-5.01340375246357
C	2.79404830705260	-0.70531395894340	-3.88094380223671
H	1.84933277165387	-2.17962693639512	-5.16156371682575
H	3.14229475711489	-1.44507550715714	-3.15394882450755

-SO₃H- Pb(H₂O)₄²⁺

C	-5.90714973185908	0.38868875650683	-0.58346290716901
C	-4.93271656231845	0.38704729654013	-1.59157208049998
C	-3.58932325017195	0.51546785657132	-1.26085049661430
C	-3.25664516349744	0.64158215161437	0.09705572087327
C	-5.55261219374465	0.52105606151156	0.76106942062597
C	-4.21112498367132	0.65146687797727	1.12008512353177
S	-1.58632127709136	0.81256104520810	0.53500623608669
H	-6.96154161629751	0.28959812065678	-0.85589895619519
H	-5.22844040535973	0.29025703424079	-2.63904107595917
H	-2.81967253379607	0.52946581820446	-2.0372967005469
H	-6.32247274393634	0.52597750988851	1.53684804490380
H	-3.91181318232410	0.75787450824227	2.16556479808977
O	-0.75630537105703	-0.20429948039877	-0.16538928529595
O	-1.40437336824782	0.92621655915140	1.97028863522445
O	-1.08025553415390	2.16113004824766	-0.18973313529478
H	-0.52920383754621	-1.92466662550696	-2.05496085575584
H	0.00048861678814	-3.72191087344171	0.91613435342826
O	0.36541046216363	-2.19148020959575	-1.79849969608033
O	0.31282378570801	-2.87608695377421	1.26873069895794
H	0.74329913846663	-2.67074793951066	-2.55155530307591
H	0.25321083243631	-2.92943378187549	2.23403803183213
Pb	1.48347846832855	-1.01677596991980	0.11850045592004
O	1.64728482892197	1.35624549932127	-0.78003825350218
H	2.41219181423303	1.84253645508848	-1.12119270471684
O	1.01547069841471	-0.27801009014336	2.45013836032996
H	1.66035438955527	0.03202771766515	3.10350521899702
H	0.87788244529929	1.94282724339723	-0.85930247683586
H	0.17964772331304	0.20320085721637	2.61581920565190
H	-1.54026144855525	2.95293450691679	0.15146899259705

-COOH- Pb(H₂O)₄²⁺

C	-6.39314209911886	0.71748999082802	-0.08463438682710
C	-5.75200724669393	1.73278414704915	-0.80253507115435
C	-4.36676793467853	1.72911690201833	-0.91584513343469
C	-3.61495396694522	0.69920946189287	-0.31941315168510
C	-5.65358055665685	-0.30256451250618	0.52433456506090
C	-4.26856049778367	-0.31492358484373	0.40950331039532
C	-2.15924772839200	0.72789501542108	-0.47033322174107
O	-1.43370734943212	-0.32695864867970	-0.10179107198246
O	-1.54876655672347	1.70243234943189	-0.93262805378218
H	-7.48317694007030	0.72159942191761	0.00552312253510
H	-6.33847887051981	2.52668842425001	-1.27123195735997
H	-3.85405643972085	2.51702386754094	-1.47188317939429
H	-6.16110659087550	-1.08561955506131	1.09246161518281
H	-3.72171979438052	-1.11463971635006	0.92260666327974
O	-0.66024035643637	2.90339565635782	-3.53593007756508
H	-1.55931375546309	2.60838101088505	-3.73939171761857
H	-0.40925432661642	3.51502517871746	-4.24495001420557
H	1.72689822087819	1.03136217077652	1.28573940370635
H	-1.37333204606455	4.18869152458306	0.05943142819907
Pb	0.63605606381731	2.32036964878665	-1.46013424300843
O	-0.45399095375444	4.22522153255003	-0.24111065319539
H	-0.09231686964256	5.06934058500274	0.06835982001190
H	0.30965456754782	-0.77709107503818	-1.95391517484462
H	0.86169601747033	-0.27691832863554	-3.31439990732573
O	0.46367384449100	0.01912867698620	-2.48201556387323
O	1.00250236913665	0.99132799658205	0.64375273178434
H	0.39595917645751	0.29534211774334	0.93604155597531
H	-1.99904937982963	-1.06201025820617	0.18934836286706

-NCS- Pb(H₂O)₄²⁺

H	-3.60206181423500	4.22967675897819	3.82235729066244
C	-3.19991011527254	3.22262683747391	3.68943645225177

C	-2.70135049368091	2.51305637988529	4.78679008136058
H	-2.71001051518894	2.97323039110721	5.77830578904020
C	-2.20078158129500	1.21685747510474	4.62968422834659
H	-1.82185086867318	0.66621197144076	5.49386920697448
C	-2.18909024534683	0.61863951027379	3.37225087612676
H	-1.81228768400460	-0.39724121031547	3.23391497769791
C	-2.68291015268638	1.34814492250595	2.28290496689916
N	-2.66427567606179	0.76421866904100	1.01370989901960
C	-3.19667307148078	2.64440061431190	2.42304980814683
H	-3.59732513177246	3.17809613506236	1.55804830816254
C	-2.63391837146457	0.28639836478857	-0.04377960619946
S	-2.66070294691072	-0.42600989507081	-1.52624509167121
Pb	-0.17003120724330	0.07244500738661	-2.50960189300551
H	0.45747308602811	2.02105542402951	0.00268502324061
O	-0.07988454896622	1.92331934946701	-0.79822857302015
H	-0.38268403038913	2.81325390357446	-1.03362348361469
H	-2.12174560910200	2.13372672694126	-3.72149987586030
O	-1.18935296912344	1.94668931684282	-3.53664268706591
H	-0.64446286506597	2.15133447392676	-4.32263995713515
H	-1.00500200894827	-2.07462260553646	-4.65417728434491
O	-1.32169765956447	-1.20925973802387	-4.34967565988049
H	-2.24754255479423	-1.16311590182884	-4.63390985563889
H	1.87697380677776	1.88542974724375	-4.69072740848479
O	1.06889437454044	1.35316566187813	-4.76406939699262
H	1.15093085392465	0.91384170951125	-5.62519613501537

-NCO-Pb(H₂O)₆²⁺

H	-2.68615968023753	3.61523066857069	5.28930451054652
C	-2.79011989142661	2.70119379115666	4.69953461067148
C	-3.33875503681513	1.55173724056215	5.27443874121685
H	-3.66494204516737	1.56719884357670	6.31733307277249
C	-3.47570770155682	0.38226143001866	4.52191597917237
H	-3.90711977364817	-0.51411362332230	4.97397334272263
C	-3.06453691437307	0.35193394733881	3.19063948478082
H	-3.16873273337668	-0.55556224574570	2.59147266471941
C	-2.51778156571012	1.51132610250348	2.63311320282420
N	-2.10202297948791	1.49427360926126	1.28816425745738
C	-2.37345046548187	2.69032785779764	3.36979483137465
H	-1.94575427659999	3.58238879864915	2.90683790198016
C	-1.76462879414121	1.50071372865394	0.17564654910918
O	-1.42700745727924	1.50612859856174	-0.99299187023870
Pb	0.27506948199647	0.84654699931663	-2.68265972709730
H	1.72892880262589	3.67247887812015	-3.05676854955404
O	0.93489630147811	3.18869525916157	-3.33438415183607
H	0.28646716874627	3.86481201232059	-3.58378513449087
H	-2.43875532162318	1.98097527578750	-3.12300674069410
O	-1.67242464045612	1.73834880872102	-3.66646469927800
H	-1.913358757725918	1.75043229244292	-4.60455909099015
H	-0.64297142752375	-2.18628452689763	-3.02122344883342
O	-0.94432333376653	-1.29687000842490	-3.26615774951949
H	-1.87778569033963	-1.39733281938363	-3.50690646635659
H	1.12006546553152	1.37283530153214	-5.64903154748542
O	0.54179865113496	0.75397863083902	-5.17625200782551
H	0.54806143475710	-0.06808485111846	-5.69098796514843

Fig. 6

-COO-Pb(H₂O)₆²⁺

C	-5.83990326581042	0.45210822025617	0.31501473865017
C	-5.17066116485772	1.44819585703757	1.03354420352742
C	-3.88890128373293	1.83487046447658	0.65211275689343
C	-3.27806672561165	1.21816161145441	-0.45154693904615
C	-5.23347927884993	-0.16171904606495	-0.78497613974770
C	-3.95077491610757	0.21795799030936	-1.17078190733917
C	-1.92243036695556	1.62319797167725	-0.86682286583777
O	-1.34739702631189	1.07663464109162	-1.86340285255742
O	-1.28400762681703	2.54514384504347	-0.24309220284833
H	-6.84675523388505	0.15079832390288	0.61690081391618
H	-5.65345774614872	1.92097424430370	1.89237427914339
H	-3.35105103692516	2.61160357105049	1.20082312437478
H	-5.76449111544541	-0.93817962625444	-1.34128184111783
H	-3.45807050212982	-0.24899191030210	-2.02637289510661
H	-1.48564660829364	4.54089298186778	-1.45854352082527
Pb	0.52117035942355	2.38224209589395	-1.69332288138755
O	-0.75446748234705	4.45187763510884	-2.08867355436666

H	-0.76418772918346	5.21819172669201	-2.67784032972775
H	0.41441453158823	1.74498016708936	1.20205350853324
O	1.15737823765573	1.66337708765808	0.58493897807156
H	1.92469598074563	1.33503214770788	1.07270552679803

-COO-Pb(H₂O)₂²⁺

C	-5.94564423777754	0.53379449202315	0.30241147670074
C	-5.09254510896618	1.25437378684509	1.14370970734060
C	-3.78485674667322	1.51881921698129	0.74364138562102
C	-3.32930550941548	1.05153210842053	-0.49829391185276
C	-5.49585429880915	0.07286220534771	-0.93820323356481
C	-4.18640270431403	0.32657836836565	-1.33952494811898
C	-1.93941415713197	1.31862660013045	-0.93223102060059
O	-1.47282349826562	0.81245717148429	-1.99482424143112
O	-1.17560530827682	2.08130703202296	-0.23726696801209
H	-6.97291593786633	0.33040326151424	0.61731836060298
H	-5.45160294246860	1.60768505217691	2.11341240559600
H	-3.10540127407838	2.08161824941053	1.38782163804775
H	-6.17034287176589	-0.48509936985165	-1.59286274292416
H	-3.81477364045374	-0.02343554426876	-2.30497495138023
H	-1.34478776382086	4.20642817262993	-1.37427935925663
Pb	0.61370627348962	1.93876065492393	-1.69145043939788
O	-0.63378884857623	4.10083686085876	-2.02280155049427
H	-0.51164820545665	4.95126803286668	-2.46464048423137
H	0.48783240615995	2.43940704992655	1.14676937301096
O	1.29812132417322	2.55056485852234	0.62546180753082
H	2.05196461098882	2.41855645560132	1.21459968139696
H	-0.12570392325492	-0.86378752600850	-1.31609915346844
H	1.34596015149295	-1.18406481725365	-0.90029095174890
O	0.69228221106733	-0.47605237266988	-0.96745187936553

-COO-Pb(H₂O)₂²⁺

C	-6.10784567796409	0.75663189466303	0.27406418881502
C	-5.30250798086349	1.75768499939022	0.82544816252681
C	-3.99843103123837	1.92747707400036	0.36772877204026
C	-3.50064090511831	1.09586011750392	-0.64605461938281
C	-5.61441345632670	-0.07350111317443	-0.73636852110361
C	-4.31130242603504	0.09466318313238	-1.19990175331070
C	-2.10487281969404	1.27660996891337	-1.12043694510917
O	-1.66362763038707	0.57205488120309	-2.08667127545746
O	-1.34384959455630	2.13026941958601	-0.56309869342373
H	-7.13086057849384	0.62177959233765	0.63589940393524
H	-5.69426313204613	2.40507178534419	1.61420128306335
H	-3.35268312207477	2.70325531525389	0.78517823022567
H	-6.24985333068257	-0.85530541132106	-1.16009197721843
H	-3.90630950647236	-0.54742594188944	-1.98527607376151
O	-0.57746021939686	1.81145592165647	-4.30022723960261
H	-1.44687726015385	1.42614782616334	-4.09724784580863
H	-0.70434755208304	2.77277912314569	-4.29440694330135
H	-0.11705156954197	1.69842462318588	0.71856487424680
H	2.71045402763842	0.32910719168486	-4.80501688073191
Pb	0.63157488402049	1.24286282406392	-2.11232489348744
O	1.91009598838853	0.68685857917078	-4.40090464809990
H	1.29999933407457	0.90200355568720	-5.12100765520297
H	-0.61715396526796	3.62877821729085	-1.62555782409966
H	1.90104593341118	2.75547148445734	0.14809132878780
O	0.12301735735004	3.66862475100939	-2.26195745887430
O	2.20179717725731	3.23388652406250	-0.65235008911185
H	3.11263557318887	3.50992628332768	-0.49133123841549
O	0.81913937438033	1.41866311594247	0.78509522571474
H	0.91260417319175	0.90348235043216	1.59625234533166
H	0.88585793549546	3.97185186377610	-1.72523123918367

Fig. 7

U₁₀-66-[OH/H₂O] defect site (Fig. 7a in the main text)

Zr	31.07975022534873	17.96328963300097	10.52189006475580
Zr	27.57222943774543	15.94665479607665	13.37333359268483
Zr	29.33237982675896	18.95763016677808	13.35683987699114
Zr	29.33306000089966	14.95748010706832	10.51447994053543
Zr	31.07013472105074	15.95174859861507	13.33438819931862
Zr	27.58655003138911	17.96364995305033	10.52052001116649
O	31.88134993543277	19.97733006378517	11.07046996097084
O	26.86848204321229	13.89995832512612	12.85271029092340

O	31.80016992136668	16.83309007207384	8.73159995115664
O	26.75940279082673	17.24293015088684	14.99856722004336
O	30.79574408342455	19.03148972497349	15.03486711644103
O	27.99465998993421	14.88487999180824	8.73683000862363
O	27.92478001045631	20.62621997808914	12.89588002391147
O	30.67138916123239	13.26947545234783	11.02673413565597
O	33.22189000568005	16.33818997307532	12.89876997188615
O	25.42469999505702	17.64135997993053	11.06453998914066
O	30.54299810393706	14.65833730525730	15.12390847424086
O	28.20845999871503	19.16485003700493	8.74887002027901
O	28.03861068827808	14.77040986779021	15.07305420048098
O	30.46136998306779	19.16536005626397	8.75104001881805
O	25.44203000640047	16.33820998332875	12.89595999472414
O	33.24060998325152	17.64053003425081	11.06665000386827
O	31.85421942439212	17.05901799263657	15.09567498885600
O	26.86765999221623	16.83160000360539	8.72986000559853
O	31.78497332888517	13.91638982444513	12.85739168004141
O	26.78576999223616	19.97888000200673	11.06913000745051
O	27.99168829355160	19.10618462315850	15.09056590924389
O	30.46136998306779	14.88635998634844	8.73645001336862
O	30.74240007154856	20.62492994890518	12.89711007080638
O	27.99453900398355	13.26364492275329	11.02378585490256
O	29.33301997463480	16.96875001725228	10.13217001229268
O	29.32388218415454	16.93423491315852	14.35727531578051
O	30.80365002456230	17.80570001347957	12.53089000992547
O	27.35348999242399	15.82721999167466	11.12411000878688
O	27.86099002292336	17.80618997877459	12.52964002164341
O	31.31220998609586	15.82720003612942	11.12522999707652
O	29.33717611282852	15.26065121830771	12.53563871062995
O	29.33315997871977	19.23804001962084	11.13406002461713
C	25.05463156774330	9.33607520176110	12.02103601464768
H	32.22101000056175	21.70664999732304	12.05952000098405
C	26.43878719571632	11.75321580287406	11.97831993303428
C	24.89413453458940	19.53329612858810	19.01283646736773
H	32.02062000361423	15.39295999793725	7.33374999934295
C	26.29732653137464	18.78254386142085	16.72214618984858
C	32.39542517005675	18.67724607142098	16.73841060265962
H	26.64815000398984	15.38914000274797	7.33364999751641
C	33.78265956000787	19.49724741132842	19.01793831085248
H	26.44571999815912	21.70786999992260	12.05963000103546
C	33.60992391409818	9.33971258619228	12.02827912068597
C	32.21626355622798	11.75809991676841	11.99502245063693
H	34.90813999786408	17.05285999654214	12.05988999998807
H	23.7560000082082	17.05559999966859	12.05829999928013
H	29.33693000007671	20.03881999632107	7.33159999507050
C	24.77829937483338	10.31039901466646	12.98292321040740
C	26.71589649089931	10.77476455792328	11.01671763600584
C	24.62728297113767	18.30363467373405	18.40557462984635
C	26.56241205520487	20.01543476079652	17.32922576457172
C	33.38320427573372	17.85321802125229	17.29148255756270
C	32.79956050937537	20.32237786245036	18.46474586328126
C	32.75566257333278	9.63738654726374	10.96265481626510
C	33.06992753406465	11.45729593459190	13.06339700200603
C	32.10702871684914	19.91557620050265	17.32511275122320
C	34.07633690496549	18.26386991162115	18.42983057216932
C	32.05550853473908	10.84366022950969	10.94679831544870
C	33.76281941559096	10.24709608620170	13.08047783389558
C	25.32752282207866	17.92795199464349	17.26079460211936
C	25.85878758310425	20.38945238135227	18.47416286501039
C	26.02183862664639	9.56542814695385	11.03887944635851
C	25.46887160437718	11.52017484978502	12.96139607375429
H	24.50663000188182	8.39186999792821	12.04231000047180
C	31.62159999699177	20.76722000278489	12.01207999144687
C	27.16308768266853	13.06573991701505	11.95134514574388
H	24.34797999867230	19.82269999689610	19.91537999879060
C	31.49503002206777	15.70881998746655	8.26243001763800
C	27.06408882169717	18.34839856294700	15.50736048436319
C	31.62968409248823	18.22975083601475	15.52730511762765
C	27.17304000987116	15.70688000482400	8.26195999655506
H	34.32119000083218	19.81940000093503	19.91496000210799
C	27.04528000929462	20.76848000660047	12.01108999050469
H	34.16071000056333	8.39353000091626	12.0410000071022
C	31.49584582991298	13.07380434676741	11.96283148526269
C	33.79136999853412	17.01864000407872	12.00910000545691
C	24.87307000334100	17.01989002244816	12.00690001530650

C	29.33533000311105	19.45055996011912	8.27338997464792
H	24.01883105176725	10.12454863605362	13.74749893698519
H	27.47470225380650	10.98241396034195	10.25880258274803
H	23.87204096995891	17.63477003158902	18.82756966272307
H	27.32458401671591	20.66570623149195	16.89327784936046
H	33.59942988417247	16.89420214883953	16.81515903802293
H	32.57248141686707	21.28751738755380	18.92547789684087
H	31.38308416888611	8.92646513569939	10.14020512826661
H	33.18085575234684	12.18630786439577	13.86938807912708
H	31.33358072813355	20.54335571203035	16.87687006653752
H	34.84843753259376	17.61997204045005	18.86002266655840
H	31.38308416888611	11.09850229958216	10.12461171549744
H	34.42860558264895	10.00992615327107	13.91494923631963
H	25.14188778665029	16.97027266208472	16.76974966717677
H	26.06338711387848	21.35205772728300	18.95070768482316
H	26.23527779299742	8.79862271858372	10.28915269028085
H	25.26268853447264	12.30149262281417	13.69634737364230
H	26.57161999908915	15.36767999901817	10.81293000325588
H	29.26540972582804	16.93751638521719	15.31480882775856
H	29.33329999762696	20.14304999923099	10.81740000132552
H	32.09310000319759	15.36673999848692	10.81295999973573
H	27.61189431344997	13.90683906964741	15.05158659937408
H	29.49799971252706	14.61424859198770	15.16148336952637
H	30.84063644110607	15.03558240094043	15.95977779504589

LiO-66-[OH/H₂O]-Pb(H₂O)₄²⁺ defect site (Fig. 7b in the main text)

Zr	31.07975068713592	17.96328979878022	10.52189062517649
Zr	27.53756674914892	15.97792599922057	13.31991635545705
Zr	29.33238017300318	18.95762997399583	13.35684013596858
Zr	29.33305962442888	14.95748004641530	10.51448023311129
Zr	31.09325555626062	15.99898111805429	13.29898722263564
Zr	27.58654984505983	17.96364946937189	10.52051989274179
O	31.88134976255988	19.97733012774346	11.07046980257963
O	26.79750473640287	13.92366344912157	12.74873034107944
O	31.80016981275131	16.83309011245785	8.73159982880890
O	26.80683756754125	17.17869140238377	15.06271710004703
O	30.73369556277527	18.99598529744718	15.05719694747883
O	27.99466007190874	14.88488001579873	8.73682993711480
O	27.92478001660806	20.62622003375924	12.89587994020041
O	30.72038421630376	13.28936412206055	11.06174423480333
O	33.22189000965555	16.33819001553941	12.89876999095220
O	25.42470001161752	17.64136005445628	11.06454003813056
O	31.21802101050521	14.63103793998305	15.32075664715213
O	28.20846001113856	19.16485009509973	8.74887002964205
O	27.42530256906176	14.59853201936838	15.06397731282098
O	30.46136995951827	19.16535998517236	8.75103993308088
O	25.44203002067828	16.33820998509262	12.89595991367523
O	33.24060994941951	17.64053008655147	11.06664999989066
O	31.85670339538754	17.07275305211713	15.08361176541027
O	26.86766004829985	16.83160007145489	8.72985997428862
O	31.78910202650055	13.91683665876380	12.92109125117140
O	26.78577004951951	19.97888007394057	11.06912997738846
O	27.97809548015148	19.07538365952074	15.06961224582522
O	30.67340006934982	14.88635998734290	8.73644995918654
O	30.74239975254217	20.62493014243281	12.89710978422403
O	28.03486586436000	13.23521298254839	11.02171302631767
O	29.33301997225139	16.96875000469096	10.13216988837306
O	29.33058070887304	16.77647107228241	14.39103857431161
O	30.80364995473618	17.80570002453653	12.53088991209770
O	27.35349006532335	15.82722005609276	11.12410994224517
O	27.86099000753790	17.80619005499979	12.52964002135034
O	31.31220999565965	15.82720003219665	11.12522993517820
O	29.32705863338885	15.13342905733433	12.60420382395456
O	29.33315995088636	19.23804005605413	11.13405992765964
C	25.05966812880997	9.32992281801712	12.02045687143139
H	32.22101002068860	21.70664999209908	12.05952001765147
C	26.43077409528625	11.74687280597004	11.94062605208869
C	24.90147630070960	19.52631509263621	19.01953257792567
H	32.02062000064776	15.39296000023189	7.33374999632289
C	26.30921042714191	18.76750653011711	16.73294195354749
C	32.37033274332846	18.68363914413544	16.74756946033471
H	26.64814999221740	15.38913999674029	7.33364999889894
C	33.77259305631424	19.50099860834049	19.02170535423396
H	26.44572000201106	21.70786999455857	12.05963000080564
C	33.62155487842754	9.34341664588124	12.03644766239891

C	32.26822578264598	11.77810528779640	12.01421035744323
H	34.90813999217154	17.05286001066999	12.05989000748276
H	23.75600000161818	17.05559999438144	12.05829999884790
H	29.33692999980186	20.03882000195518	7.33159999802657
C	24.59027228848741	10.41339172845697	12.76809508050499
C	26.89400801373142	10.66095957220653	11.18753245643473
C	24.54668244941724	18.35474265603855	18.34293365603770
C	26.65498394204967	19.94692562174034	17.40605239981053
C	33.42247509615039	17.90006257519846	17.24610819178985
C	32.73150786479836	20.28938512572472	18.52200234548155
C	32.60315005808995	9.56167390299694	11.10447019729099
C	33.29406781816141	11.55514130176798	12.94684579081368
C	32.03239049283229	19.88633958377912	17.38487533507864
C	34.12074195878333	18.30799900258351	18.38038345174889
C	31.92758920546149	10.77987815809369	11.08858674754250
C	33.96861066102479	10.33701340144603	12.95699954896226
C	25.24843292017250	17.97528056469914	17.20136660149276
C	25.95131960837794	20.32133311910768	18.55099430092674
C	26.20844718650307	9.44784275544774	11.23454632023879
C	25.27601910172726	11.62422319655069	12.73090576919698
H	24.50663000906600	8.39187000807625	12.04230999502039
C	31.62160023005720	20.76721985684438	12.01208020546521
C	27.14148847580547	13.05501710823699	11.88908040295632
H	24.34798001118750	19.82269998720641	19.91537998030497
C	31.49503007799976	15.70881995554218	8.26243005216625
C	27.07015491408384	18.33369278137417	15.52415021374505
C	31.60918441793605	18.23889520700991	15.54684794268777
C	27.17303993802263	15.70687998538005	8.26196005216676
H	34.32118999188253	19.81939999610401	19.91495998814703
C	27.04527994969078	20.76847995759278	12.01109007473751
H	34.16070998279113	8.39353002298720	12.0409999974936
C	31.55118930205045	13.08194598245978	11.98008099836878
C	33.79137000540885	17.01863992210171	12.00909996082954
C	24.87306999500537	17.01989002059860	12.00690005390395
C	29.33533000613760	19.45056001139475	8.27339001530437
H	23.67356626117409	10.31489162881901	13.35548947703800
H	27.78137441653354	10.78701787756637	10.56282587964100
H	23.70901879906890	17.74990849883834	18.70038300877625
H	27.47228639620237	20.56142511876267	17.02098961359763
H	33.70404969571063	16.98172075930953	16.72568012359302
H	32.47057629212956	21.22765338412069	19.01786334318522
H	32.34410989829552	8.78252644313008	10.38330434982088
H	33.57723414688782	12.35130098603031	13.63959882680721
H	31.22199350267784	20.49599085950903	16.97856638287081
H	34.94644776129894	17.70176021616124	18.76167925246734
H	31.14168444489389	10.98044581371379	10.35662539828924
H	34.77787134136761	10.16148697211966	13.67043760364839
H	24.96926306943785	17.07875777771719	16.64153420308073
H	26.21554663491640	21.24218934753090	19.07679998370059
H	26.55897724162897	8.59606871394741	10.64662360193388
H	24.90584732370800	12.49597993819645	13.27631753338204
H	26.57161999682531	15.36767999296751	10.81292999644388
H	29.32649792759636	16.85274755478362	15.35263485979972
H	29.33330000316085	20.14304998824420	10.81740002570680
H	32.09310001748622	15.36673999984887	10.81295999026832
H	26.91589903200040	13.89676108696487	14.62056409063921
H	31.74721601047510	15.27294640834955	15.83406277660454
H	31.82010964197987	13.94661954946102	14.97843323901055
H	26.32354907929150	11.41674158212025	15.81227562643969
O	27.17029729971075	11.72013102098959	15.45891359609555
H	28.52779476707029	16.59804646008576	17.84878627973491
H	27.22243172196682	11.41517953304717	14.53903349683985
O	28.53207308779128	16.06409337330195	17.04217547832780
H	27.69909762345265	16.26553187367553	16.56856111760992
Pb	28.76253454028276	13.47640580321971	16.35386288779579
O	29.30809560507822	12.69461588140070	13.97877884647145
H	29.96048738450968	12.05890778113550	13.65447750747021
H	25.94074375413942	14.24140832175555	17.30419968249867
O	26.51679244906774	13.54857946970297	17.65837032737314
H	29.33795915211494	13.47364122790863	13.37262569957278
H	26.29253177567509	13.45678649449381	18.59460453337972

U₆O₁₃-[OH/H₂O]-Pb(H₂O)₆²⁺ defect site (Fig. 7c in the main text)

Zr	31.07974952454170	17.96328975799866	10.52188934534051
Zr	27.61296505623893	16.00287449168295	13.33717479122477

Zr	29.33238015383617	18.95762993874172	13.35684022993195
Zr	29.33306006840956	14.95748015310650	10.51448014755038
Zr	31.11085524043814	15.98741840282236	13.32866219082890
Zr	27.58654997723393	17.96364950460095	10.52051968553302
O	31.88135012645870	19.97732998374705	11.07047011219591
O	26.94768123449577	13.83521901649941	12.92090415877476
O	31.80017007335465	16.83308999339899	8.73160011246070
O	26.78544922532149	17.12441620661806	15.05549480876778
O	30.74724623568431	19.00877730913663	15.05393902063961
O	27.99465999483370	14.88487999640718	8.73682998606926
O	27.92477999167784	20.62622000370493	12.89587999019815
O	30.64713148113247	13.26460229022345	11.03944972973406
O	33.22188998349126	16.33819012477093	12.89877010319529
O	25.42470001908003	17.64136014319321	11.06454008926807
O	30.60836991377095	14.70548467761893	15.27429199431145
O	28.20846001680615	19.16485022561359	8.74887014679787
O	27.91271943480378	14.77592092218842	15.21103174143084
O	30.46137002184069	19.16536014522413	8.75104014211451
O	25.44203000848894	16.33820996036975	12.89595998513589
O	30.64713148113247	17.64053016951778	11.06665015401275
O	31.84480415546352	17.06571060362663	15.08957236300075
O	26.86766000623131	16.83160002839028	8.72986001515419
O	31.64933501671402	13.85796379997982	12.94693159282382
O	26.78577000706248	19.97888003687544	11.06913000739206
O	27.92994160839665	19.03821831209017	15.06136904464230
O	30.67339991969037	14.88636003314615	8.73644991895364
O	30.74239990061249	20.62493004422929	12.89710991694121
O	27.97050367948757	13.25436707725227	11.01519030626714
O	29.33302006003842	16.96875004045025	10.13217007916928
O	29.33468920603395	16.91424174606559	14.36313593849745
O	30.80365008818504	17.80570005449789	12.53089008495319
O	27.35349000876903	15.82722005512770	11.12410995943259
O	27.86098998746054	17.80619003047188	12.52964000637579
O	31.31221001014771	15.82719998540374	11.12523004290058
O	29.33064061621914	15.22838347909405	12.58058761969124
C	29.33316004130827	19.23804005434339	11.13406003883006
C	25.04953665558478	9.33428545716224	12.01998493956513
H	32.22101000067740	21.70664999746424	12.05951999978278
C	26.41783194066537	11.74835270094505	11.94943513024782
C	24.88744869863175	19.51333501554216	19.01533925215715
H	32.02061999659328	15.39295999993430	7.33374999472794
C	26.27443057727328	18.72180781758554	16.72845116378422
C	32.38851616731976	18.68778532501722	16.73572107566273
H	26.64815000044906	15.38914000159568	7.33365000030871
C	33.78044585921344	19.50160095070208	19.01611790001720
H	26.44571999722630	21.70787000098889	12.05963000056235
C	33.59566617997078	9.33306748737981	12.03718335928653
C	32.17928431954506	11.74168689553183	12.01604726395102
H	34.90813999949307	17.05285999128212	12.05989000119643
H	23.75600001273005	17.05559999275838	12.05829999166948
H	29.33692999996437	20.03881998188783	7.33159999595245
C	24.51740477089558	10.44429630062557	12.67841984508381
C	26.93400219782178	10.64259691159881	11.26009301440416
C	24.62265494003525	18.26632191436137	18.43970431644687
C	26.53298904632531	19.97301789473780	17.30383256200664
C	33.39659338335512	17.87222205809351	17.27206404442202
C	32.78377354214287	20.32100265326104	18.47701099137731
C	32.74874946682841	9.63526047345810	10.96549238640382
C	33.03160349103133	11.43747536029705	13.08886812707047
C	32.08878266743597	19.91889765706193	17.33767417514590
C	34.08994040165584	18.27968754673541	18.40999465963751
C	32.03924573715922	10.83554475795388	10.95354205766387
C	33.73345369528495	10.23258357775157	13.09965728738721
C	25.31406721726317	17.87208235246245	17.29747130946209
C	25.83756502708714	20.36569658135437	18.44663615131099
C	26.25217912452881	9.42729303422188	11.30927935482643
C	25.20327850488323	11.65744508163519	12.64699910383590
H	24.50662999728450	8.39186999890962	12.04230999965992
C	31.62160000851378	20.76721999396633	12.01208001256453
C	27.17123294235923	13.03143019822416	11.93468314370005
H	24.34797999835836	19.82269999725951	19.91537999836796
C	31.49503002657447	15.70881998349762	8.26243002264601
C	27.03968481430120	18.28219367309634	15.52905172573148
C	31.61974090615357	18.24063348036294	15.54183438681240
C	27.17304000714274	15.70687999871609	8.26196001049737

H	34.3211899997716	19.8194000046303	19.91496000092086
C	27.04528000672116	20.76848000463335	12.01109000362967
H	34.16070999720119	8.39352999776978	12.04100000108922
C	31.44835250443206	13.04242275269555	11.98868969820925
C	33.79137000834901	17.01863980106225	12.00909984963093
C	24.87306996589427	17.01988997607450	12.00689995607247
C	29.33532999311075	19.45055979144601	8.27338985885856
H	23.56051173810916	10.36576404886412	13.20003595960123
H	27.86491663794042	10.75064178451049	10.69807373372089
H	23.87400375461976	17.60645552267198	18.88610022593698
H	27.28092940173250	20.62579659609371	16.84784119885514
H	33.63628868736459	16.92469620123451	16.78397138444763
H	32.55056794578167	21.27938732056253	18.94751406803489
H	32.65213262431251	8.93619177785010	10.13053863320162
H	33.14997853254093	12.16190817923646	13.89836426741940
H	31.30885491282011	20.54927048267939	16.90444951611430
H	34.87858292083181	17.64648160052387	18.82462260544817
H	31.38714687011477	11.09381977639932	10.11595699121104
H	34.40423464898821	9.99755612548049	13.93021517700474
H	25.12116809369784	16.90395661038966	16.82965882595591
H	26.03573401950298	21.34127875587973	18.89726358314855
H	26.64263221586672	8.55581093803080	10.77732234452490
H	24.78140628525821	12.54384564475935	13.13093520648377
H	26.57161999115615	15.36767999023606	10.81293000259907
H	29.33170651682969	17.08163839584685	15.30709442987086
H	29.33329999918654	20.14304999950414	10.81740000134675
H	32.09309999799475	15.36674001026177	10.81296000286657
H	27.50416111828837	15.32361107737091	15.89800986562270
H	29.62685944713136	14.74482039565803	15.40932606356130
H	31.02535108599625	15.19772791531979	15.99660428932891
H	28.15308222910863	9.23134188332469	14.79738539272834
O	24.90999116006863	14.45234709578343	14.90458419113264
H	24.27203595455093	14.71749482980038	15.57919136883386
O	27.95397269085112	10.01598896566132	14.26813943529249
H	27.48466934588028	9.67947539107515	13.48785082203951
Pb	26.97087571665411	12.74076565561522	15.10372745189851
O	29.29110671283532	12.32126809448109	14.36118420274997
H	29.34835028778937	11.41486864192512	14.01248066995283
O	28.61226897556563	12.58780516850717	17.15928163827264
H	28.65454159612974	12.18114516543295	18.03498147770439
H	30.02494664434194	12.86904848191708	14.02948888399257
H	29.46809923517317	12.42278691068317	16.73586407699919
H	24.87709050331747	15.15638800660488	14.22138120732254

U_iO₆-[OH⁻/H₂O]-Pb(H₂O)₂²⁺ defect site (Fig. 7d in the main text)

Zr	31.07974967459521	17.96329021605425	10.52188979270712
Zr	27.51164378981978	15.94063230260525	13.31976178883370
Zr	29.33238033920665	18.95763003019664	13.35684010074064
Zr	29.33306028658310	14.95747991899571	10.51448023217828
Zr	31.11299186493715	15.97546352953914	13.29435736437591
Zr	27.58654992811316	17.96364951457556	10.52051961048465
O	31.88135003622247	19.97732999522297	11.07046998099857
O	26.92241729554562	13.86660608710807	12.80389500592251
O	31.80017003169211	16.83308997169910	8.73160003026247
O	26.72885751104538	17.20089972726857	15.01512657292704
O	30.64253939649081	18.98599514220006	15.10525055916085
O	27.99465999483687	14.88488001126302	8.73682998050215
O	27.92477998389104	20.62621996921075	12.89588003406018
O	30.70996077809999	13.27779958333050	10.99059354472288
O	33.22189001387152	16.33819000384768	12.89877001566515
O	25.42470000147065	17.64136015009720	11.06454007880351
O	31.87979184937918	14.78852972235190	15.24001026903218
O	28.20846002627682	19.16485024176026	8.74887016092559
O	27.38655513463409	14.69612016645311	15.09751016242566
O	30.46137001384039	19.16536003659560	8.75104005358244
O	25.44202996965213	16.33820995149591	12.89595995398482
O	33.24061001349018	17.64052999659103	11.06665001980808
O	31.95076851835396	17.20860767093104	14.99944319658054
O	26.86766002798787	16.83160004617861	8.72986001335501
O	31.64556869307759	13.83056077744328	12.93764361063815
O	26.78577003980382	19.97888007482369	11.06912997054373
O	28.05287023019621	18.97568763534712	15.10938360678995
O	30.67339987554540	14.88636005330688	8.73644990847281
O	30.74239984279587	20.62493004387762	12.89710993949646
O	28.04963763072671	13.23678407165474	10.99008587443515

O	29.33302001120055	16.96875003535385	10.13216997661320
O	29.38129471700443	16.50824087135224	14.63868633470650
O	30.80364990716988	17.80569988017450	12.53088999101505
O	27.35349000859288	15.82722011712944	11.12410995927515
O	27.86098990987096	17.80618999118678	12.52964000365213
O	31.31220998015712	15.82719999921870	11.12523001493456
O	29.32979782856586	15.24195350707109	12.58962949247484
O	29.33316003924279	19.23803999882799	11.13406002671358
C	25.05035973297557	9.33628534488575	11.99124858100281
H	32.22101000592718	21.70665000789479	12.05951997755486
C	26.43067597506057	11.74783895765040	11.89428197023923
C	24.28339619616383	19.54750723729171	18.99906110449362
H	32.02062000133768	15.39295999939126	7.33375000221967
C	26.27052183040685	18.80283744838275	16.68679663842371
C	32.41373481320834	18.79372907206353	16.69129530005053
H	26.64815000042500	15.38914000126429	7.33364999777048
C	33.79020560355315	19.54399670674966	18.99878947244970
H	26.44571999765380	21.70787000791108	12.05962997653082
C	33.61870380512611	9.33829067555370	12.01127089889041
C	32.23388554099476	11.74954669316412	11.96315564953666
H	34.90813998823590	17.05285999241051	12.05989000645002
H	23.75599999417016	17.05560000313913	12.05829999277562
H	29.33692999818694	20.03881998024527	7.33159999996182
C	24.66743757566310	10.38471953361074	12.83187079221026
C	26.80075109967376	10.70125395183030	11.03913858716413
C	24.35545515095890	18.56481495844254	18.15456081863829
C	26.78109336062046	19.81256616973766	17.51467830780987
C	33.58324233292181	18.11295618720891	17.06621619648416
C	32.64176964014670	20.24262195816673	18.61465057707601
C	32.77449953105190	9.62925856212915	10.93678033546875
C	33.09243163488546	11.45420494011082	13.03348501771991
C	31.95419612963386	19.87356963061547	17.45876296225692
C	34.26963336205954	18.48849506716639	18.21690443812846
C	32.07832508319375	10.83541918673795	10.91086156549009
C	33.78218734469618	10.24772531405692	13.05936305272380
C	25.04516830399962	18.19141127574758	17.00282103698676
C	26.08999192229098	20.17679843433454	18.67223069365003
C	26.11060139543935	9.49152731874220	11.09409706915472
C	25.35850376488756	11.59069940828271	12.78676918808615
H	24.50663000842652	8.39187001138231	12.04231000009634
C	31.62160008915993	20.76721995596877	12.01208010610331
C	27.18031219429271	13.02820703426721	11.87658021934729
H	24.34797998530851	19.82270000564692	19.91538001918011
C	31.49503003615898	15.70881997391658	8.26243004880267
C	27.04874833472293	18.31555449559021	15.50956762277806
C	31.63806851567734	18.32323833107165	15.51540883953428
C	27.17303998277740	15.70687999069285	8.26196003224235
H	34.32119000142124	19.81940000138069	19.91496000286518
C	27.04527996886962	20.76847999570805	12.01109004256345
H	34.16070999623672	8.39353000690202	12.04100000080295
C	31.48290820175395	13.02670269143324	11.93897468775085
C	33.79137000501665	17.01863999856458	12.00909998351720
C	24.87307001570312	17.01988998375605	12.00690002114070
C	29.33532999527792	19.45055985703001	8.27338991408905
H	23.82458056234310	10.25616469170694	13.51587703103031
H	27.62986892057877	10.84831385146755	10.34293684981839
H	23.39950723834037	18.09263939777397	18.39465849488808
H	27.72366939727647	20.29634170505855	17.24772740594103
H	33.96003537746194	17.29916817458195	16.44195167037235
H	32.28280592997165	21.07858934543660	19.22016289656522
H	32.66032317125209	8.91284196068703	10.11939001049895
H	33.22505559911431	12.17582753802110	13.84154858240959
H	31.05359847527208	20.40700122451484	17.14580208982609
H	35.18219456012793	17.96208148755825	18.50711760717023
H	31.41195853756875	11.08485932964147	10.08224128355653
H	34.45176619366237	10.01082995018059	13.88985427725965
H	24.63820011916227	17.42842150177142	16.33349025173779
H	26.49232530103463	20.95658208978419	19.32394315120888
H	26.39614439629529	8.66761434129409	10.43553123402080
H	25.06537249629641	12.42497392439252	13.42794120096858
H	26.57161996932383	15.36767997840395	10.81293001640865
H	29.43177660527016	17.20449718899103	15.30758105564237
H	29.33329999761105	20.14305000144982	10.81740000053830
H	32.09309999392073	15.36673999346732	10.81296000917626
H	26.93579195021743	13.85856435814162	14.92837735754057

H	32.37985892076424	15.53490105848883	15.62721715965282
H	32.51178982378990	14.13119948441730	14.90952350436540
H	26.84975181131200	13.18708354163288	17.78351988230150
O	27.57256089430497	12.82908914431846	17.24658818558045
H	27.03373011625683	16.55763346550555	18.12684470637560
H	27.71073994337299	11.91422193062426	17.52862299870647
O	27.19194757934015	15.82357974859078	17.51576546457980
H	26.68061326325103	16.03148403213208	16.70911682933711
Pb	29.13168297902385	14.61133921230828	16.41395775196893
O	29.55748094477843	13.00550667329272	14.58430533951465
H	30.40241864008526	13.09574741643583	14.10116540446236
H	28.88305635871848	13.19606442198553	13.91145883513940

UiO-66-[OH/H₂O]-Pb(H₂O)₂²⁺ defect site (Fig. 7e in the main text)

Zr	31.07975002304768	17.96329011442456	10.52189015870022
Zr	27.51138604776373	16.02613001691746	13.36473889899530
Zr	29.33238021348405	18.95762972618718	13.35684015863815
Zr	29.33306010998023	14.95747998431251	10.51448011050836
Zr	31.12939602649325	16.03306035371498	13.32184602577692
Zr	27.58654992177255	17.96364970271564	10.52052000439179
O	31.88134993475663	19.97733002105042	11.07046994208637
O	26.92691012592679	13.81458259420383	12.82878010405866
O	31.80016998013518	16.83309001848542	8.73159995154345
O	26.77763335094200	17.16546693373622	15.02337828439740
O	30.76479398041731	19.00954141729019	15.03379131104555
O	27.99465999120112	14.88487998754419	8.73683000032132
O	27.92478003191441	20.62622009546694	12.89587991251236
O	30.67383920011853	13.27160271455844	11.08759472078640
O	33.22189002048359	16.33818994462678	12.89876995037924
O	25.42469998333370	17.64136006877446	11.06454000144319
O	31.04980115160415	14.55591716963482	15.26803517962846
O	28.20846000969069	19.16485007470031	8.74887001803733
O	28.00707871537981	14.72469093854417	15.07859285815451
O	30.46136999840617	19.16536003045246	8.75104000346306
O	25.44203001715877	16.33821006352715	12.89596004326015
O	33.24060998658427	17.64052989349533	11.06664993250930
O	31.84663563040449	17.06222303404633	15.08796793742531
O	26.86766004782457	16.83160005603524	8.72985994190539
O	31.73657046981293	13.89529116428507	12.94519594118994
O	26.78577004604273	19.97888004625349	11.06912996023282
O	27.98115213692958	19.03404535221267	15.07228058323441
O	30.67339992682364	14.88636000155445	8.73644996066548
O	30.74239985977866	20.62493013832136	12.89710985412521
O	27.98543224602713	13.23859236689657	10.95467257640158
O	29.33301998861124	16.96874996653703	10.13216996091071
O	29.34590411615459	16.85177605987206	14.35271246435590
O	30.80364995995861	17.80570009228818	12.53088995388412
O	27.35348998725795	15.82722003239828	11.12410999887181
O	27.86098997768309	17.80619015561190	12.52963996395231
O	31.31220997203433	15.82720000558955	11.12523003260269
O	29.32382192451607	15.11020808863053	12.64298093914571
O	29.33316001115589	19.23804005842635	11.13405993655748
C	24.99182930897908	9.36015571721352	11.94613475891803
H	32.22101001011641	21.70664997486168	12.05952003331986
C	26.28528692961184	11.80337201775774	11.76727487739051
C	24.89544556747665	19.52025761576017	19.01462660541383
H	32.02062000907708	15.39296001614630	7.33374998297414
C	26.29770458260950	18.73792528162814	16.72898954081734
C	32.38356321647117	18.68608445888836	16.73770866834382
H	26.64815000490944	15.38914001486541	7.33364997983892
C	33.77791434714565	19.50148199316764	19.01729308822993
H	26.44572000084232	21.70786998981120	12.05963001934966
C	33.63499506292956	9.35162730474342	12.02238951180986
C	32.28403727861623	11.78852442411610	11.99067967820944
H	34.90813998467420	17.05285999078098	12.05989000994115
H	23.75599998889272	17.05559998743816	12.05829996558481
H	29.33693000379288	20.03882001252297	7.33160000920532
C	24.47169320583629	10.46408365445661	12.63222547814797
C	26.77091834722860	10.70993964349038	11.03953803253395
C	24.59718500649647	18.30110410338926	18.39749662237739
C	26.59005183886164	19.96430570510336	17.34431088919128
C	33.41629792519553	17.88783534426960	17.25460784308876
C	32.75579437840611	20.30318201715085	18.49952774662876
C	32.75082612880765	9.64103627385558	10.97872579537979
C	33.18564561569368	11.49956547106579	13.02837322851359

C	32.06013268299144	19.90119959534847	17.36048371439422
C	34.11092816901721	18.29571703179858	18.39104829424939
C	32.07197326384436	10.85716022467422	10.96134953980345
C	33.85621447063335	10.27980793614198	13.04518677072593
C	25.29499841367623	17.90977261329486	17.25755141802566
C	25.88826352426653	20.35130693590858	18.48526777213331
C	26.12317087735413	9.48055535876430	11.13928607544072
C	25.12238406913930	11.69099030214739	12.55043199402232
H	24.50662998205819	8.39186996420219	12.04230999433651
C	31.62160008825413	20.76721992088938	12.01208009142720
C	27.08729744327691	13.04404398206527	11.80772444595691
H	24.34797999868149	19.82269999533665	19.91537999559318
C	31.49503006058536	15.70881997514040	8.26243004141451
C	27.05947992503467	18.30012939706429	15.53075480690955
C	31.62139309708979	18.24445839906900	15.54081601700407
C	27.17303995137401	15.70687998136249	8.26196003021499
H	34.32118999582840	19.81939999773502	19.91495999688628
C	27.04527992303253	20.76847994239951	12.01109007212491
H	34.16071000175381	8.39352999758106	12.04099999969692
C	31.53513696636826	13.06706662003254	11.98600845442283
C	33.79136999960122	17.01864010149447	12.00910007338967
C	24.87307000181827	17.01988994033960	12.00689999745201
C	29.33533000103047	19.45055994930196	8.27338996895898
H	23.55953803243377	10.35969177230883	13.25232323123613
H	27.66597741029662	10.83087177979878	10.42493055645152
H	23.81567131729384	17.65637265288073	18.80766643549273
H	27.36781403738166	20.60418402091858	16.92091341325387
H	33.67941802796481	16.95553866096960	16.74985251368782
H	32.50295450560090	21.24821616863239	18.98640180127010
H	32.59308352110254	8.91491286619956	10.17728913342964
H	33.36597841980431	12.24045507267680	13.81048607492293
H	31.26106688502369	20.51922767717237	16.94479929392126
H	34.91929196427380	17.67693543725372	18.78890148430592
H	31.37847524281164	11.10241221028271	10.15394565768491
H	34.55906792841100	10.04886641616397	13.84961839900816
H	25.06940000878483	16.96189742493544	16.76457338647260
H	26.11405338898424	21.30673740409590	18.96519952556447
H	26.50352062174904	8.61249913207865	10.59566298221589
H	24.73322543494245	12.57167078197408	13.07090161940338
H	26.57161999784616	15.36767999758982	10.81292998157861
H	29.26290712021623	16.91207058658059	15.30801670807491
H	29.33329999650370	20.14304998725119	10.81740001307975
H	32.09310000421641	15.36673998896394	10.81295998111186
H	27.27933403469089	14.32818577357862	15.57688034184467
H	31.11731981179440	15.11785296234620	16.05792514997303
H	31.87740416191131	14.05147511746569	15.2048087784557
Pb	29.08964339661807	13.17264737033790	13.96418643896945
O	27.07019801302992	11.95764951196081	15.13648003111498
H	27.05709785861994	11.19580808125165	15.73244129477014
H	26.33150811538994	11.81733585153588	14.52083211275851

Supplementary Material:

Table S2

<u>-NH₂-Pb(H₂O)₆²⁺</u>			
O	1.14931814887374	2.02089629958856	-2.02670480130539
H	0.90845632037630	2.91571615312769	-2.30086768772128
H	1.32935975306356	2.02132453755518	-1.06101462215737
Pb	0.57285339622109	-0.36115836194316	-2.30180555342733
H	3.80464580876146	-0.71279874387611	-1.52344798415834
O	3.02011055957032	-0.99918499070228	-1.02255933186683
H	3.25320440544081	-1.87521289062618	-0.68040639739722
H	-2.69958992241925	-1.54854362639740	-1.23714923600146
O	-2.22921946741920	-0.70067458627746	-1.22988256006101
H	-2.54584489918511	-0.26235283135947	-0.42508901483335
H	-1.71605288618399	1.34356946894517	-3.89101553539514
O	-1.44142276023355	0.52026013531684	-3.46457631139394
H	-2.12850475825792	0.27460539236761	-2.81036724524998
H	-1.02180028006390	-1.84154256887995	-4.60669554306508
O	-0.24068959508838	-2.10885176006230	-4.09914023900519
H	-0.19674280517510	-3.07371661311691	-4.17140946809237
H	2.18597266813572	0.24424796637456	0.24029375768082
O	1.36529845941502	0.77097297303260	0.25867507892756
H	1.16351467878318	0.94635090023251	1.18829579658341

H	4.99346408450702	-3.11840104133211	-4.07439341798855
H	2.72337407117127	-2.32898055139984	-4.71888237987703
C	4.72210829591690	-2.06945877819456	-3.92869017092000
C	3.44788670711063	-1.62770331976643	-4.29326318877621
C	5.65440436154504	-1.17356490580088	-3.39756062553925
H	6.65526842421189	-1.51915096758543	-3.12693745214598
H	1.33992458304301	-0.39684562088204	-5.15588378941078
C	3.11186946386017	-0.28091935513925	-4.12938585912009
N	1.76278708423133	0.15336156046301	-4.40634472845010
C	5.31005182376446	0.17328340050072	-3.23972772361454
C	4.03545991201939	0.62397603207340	-3.59905707592592
H	1.73481070127152	1.13750831075882	-4.67529028107706
H	6.04224071439253	0.88389657168513	-2.84635306974693
H	3.76749294833894	1.67676181132014	-3.47187333946642

Fig. S3

-COO-Pb²⁺

C	-5.81200917177359	0.27234405394436	-0.21481512341132
C	-5.08212821419947	1.07345586877601	0.67080318947882
C	-3.76393414292681	1.40394353239499	0.37760354209480
C	-3.18052449640269	0.92351618064063	-0.80967545817396
C	-5.23349245550446	-0.20537733997856	-1.39611392221032
C	-3.91598792414874	0.11735562305392	-1.69875193423434
C	-1.80188553240599	1.26225698905570	-1.12500514620181
O	-1.22712000635597	0.84592119293654	-2.20335237943571
O	-1.07965561906448	1.99556613845858	-0.34709402517451
H	-6.84901667180273	0.01618891861492	0.01955348810149
H	-5.54756184982297	1.43738530245155	1.58971737281493
H	-3.17652881732396	2.02848972477592	1.05459869429867
H	-5.81513771507951	-0.82933230203328	-2.07898726747219
H	-3.44457023783688	-0.24434923101348	-2.61502236595846
Pb	0.66647285464828	1.86600534792218	-1.69760866451607

-NHCSNHCH₃-Pb²⁺

H	1.28963664997791	-5.17837974825901	-1.07187634753189
C	0.46996184344100	-4.77845233321034	-0.46675906950155
H	1.32929351703558	-5.42123749561808	1.41531080977610
C	0.48996387319576	-4.91651751073777	0.92796845535626
C	-0.61860689420073	-4.15098030258619	-1.10415238158535
H	-4.82041815180175	-2.95575812820311	-3.00922319970238
C	-0.56330672169944	-4.40559361757915	1.69907832531231
H	-0.65590745822988	-4.07107933015657	-2.19564088348758
H	-0.55094518192248	-4.51533198852840	2.78815216057247
C	-1.65980822597852	-3.77459617145607	1.07847657576913
C	-1.69208890551831	-3.66061896709487	-0.32877268753709
C	-5.16235020889127	-2.17858207745633	-2.30700762020445
N	-2.82265041839018	-3.06823082913431	-0.97216602983846
H	-2.50043760318883	-3.40129454495748	1.67228876457823
H	-3.57826103075046	-3.70092918944379	-1.23373436081385
H	-5.66071781851039	-2.63185079611861	-1.43519298745113
H	-5.88983189901696	-1.54407345288122	-2.82718457695555
C	-2.95777486647837	-1.76015786411833	-1.26503693390915
Pb	0.20879354856886	-1.76462370325510	0.25815556888917
N	-4.03922187265736	-1.33657965329000	-1.88301065315139
S	-1.75754014197951	-0.55726866468310	-0.86674100714824
H	-4.09001203300454	-0.33750363123200	-2.07633192143556

-SO₃⁻-Pb²⁺

C	-6.10439902957720	1.07172656190307	-0.08034286971429
C	-5.30896007274625	1.88673799222929	0.73426679009965
C	-3.93838515811576	1.66504892186494	0.81207670657768
C	-3.39050422001154	0.61859378307230	0.06211022708770
C	-5.54033826719512	0.02615445518478	-0.81283280461256
C	-4.16769032736134	-0.21354208522089	-0.74712119998902
S	-1.67206102372493	0.31302732373137	0.09805554506743
H	-7.18120506485514	1.25295699750496	-0.13733368491452
H	-5.76323962240539	2.69271529438132	1.31546494671613
H	-3.31626757791788	2.28213852426632	1.46472894915057
H	-6.17044487346776	-0.61161355863402	-1.43743383756053
H	-3.70567299755230	-1.03249982188655	-1.30296640429678
O	-1.34707009909466	-0.99115366074504	-0.40554574802359
O	-1.17010213736551	0.61694463494734	1.54025845928067
O	-0.95377286408866	1.47868970807480	-0.65703386228153

Pb 0.25583333547949 2.21374492932600 1.01103878741299

-NH₂-Pb²⁺

H 2.58253199531551 0.52401146085728 0.95408071923767
C 1.67544758569954 0.31638030920903 0.38003074842007
C 0.432029444860786 0.28614786986380 1.01808781249816
H 0.36116087856236 0.47292377363624 2.09454366677162
C -0.74576953380204 0.00574500595117 0.29304286566773
H -1.70723761773950 -0.07406126339607 0.81606902949843
C -0.64908889271526 -0.30822739520818 -1.08398258468107
N -1.84809823330463 -0.33377938527959 -1.86666959031663
H -2.67703005912299 -0.68626447532558 -1.37665999721838
H -1.76535714494500 -0.81371755980870 -2.76900849578964
C 0.59489987359654 -0.19905892321326 -1.74949990596098
H 0.67742081164408 -0.43591537866433 -2.81771621039542
C 1.75412901945273 0.08335883425588 -0.99583809661388
H 2.72341377664499 0.11096012469141 -1.50372040342136
Pb -1.15444190789420 2.02656700243089 -1.63509955769631

Non-functionalised UiO-66-Pb²⁺

Pb -1.46832248739021 -0.42863192380156 -3.02198510391779
C -1.27928327991664 -0.67679889219863 -5.75391704272327
C -2.44693929204885 0.09386415133448 -5.53432323539289
C -1.20340728866274 -2.00331137074513 -5.26358535284002
H -2.51377692929256 1.11261179291562 -5.93371765313329
H -0.30825230312564 -2.60690706845520 -5.45481953876060
C -3.53921961321302 -0.46333150030114 -4.82525921025519
C -2.29536212352857 -2.56007061416994 -4.55374874789096
H -4.45225607334529 0.12469965694141 -4.67479329396116
H -2.24612539429699 -3.59429531763969 -4.19338805775462
C -3.46285120130931 -1.78937362129940 -4.33364191566543
H -4.31660802950867 -2.22670940418429 -3.80278278829130
H -0.44255598436150 -0.25458588839651 -6.32292805941341

-SH-Pb²⁺

Pb 1.57029116816417 -0.00069600332203 -2.28410033403692
H 4.51829008916923 -3.01433630442246 -3.08806670101063
H 2.66918977164975 -2.19636003710548 -4.53452668616658
C 4.36649350085255 -1.93579941431728 -3.20101201269648
C 3.30649060697649 -1.47562031892096 -4.00861742302236
C 5.22070384408702 -1.03313595929233 -2.55753938629223
H 6.04282222339801 -1.40428398518397 -1.93854782636267
C 3.14891204921313 -0.08277669977670 -4.20419468450750
S 1.69332735952728 0.62010367994292 -4.98942350640529
C 5.02514560573322 0.34381515959618 -2.70920117791958
C 3.98186549282420 0.83677081335612 -3.52008125726226
H 5.69406963608505 1.05371547020937 -2.21198386671431
H 3.87273861873243 1.91658109294989 -3.68310237869970
H 1.20515003358739 -0.50986749371326 -5.55491275890345

-CONH₂-Pb²⁺

C -4.45659470929132 1.64985277874175 -1.77470938017813
C -3.52450315704245 2.25072878314164 -0.91432511805485
C -3.04988392022575 1.54647462994826 0.17666117973921
C -3.51330464043963 0.21771709104671 0.41631503236019
C -4.92617936754176 0.34092290413558 -1.55358927903072
C -4.46388467357473 -0.37604747963757 -0.46859652624377
C -3.00488560988629 -0.47539655836248 1.53436008561719
N -3.40767069967536 -1.83422667820853 1.90304417029402
O -2.14978235106395 -0.02121789468494 2.35378923821153
H -4.82821116237849 2.21075977514287 -2.63819110922101
H -3.17755106068571 3.26852990015200 -1.10660656225260
H -2.32375982316401 1.99558868139687 0.85865017839247
H -5.65251744732217 -0.10167045810807 -2.23940210298162
H -4.83507140170500 -1.39223004419738 -0.30823345723365
H -3.18461902515451 -2.51281706843021 1.16200147372693
H -4.42379739680049 -1.90884793625545 2.04822712451882
Pb -1.86285355404820 -1.63137042582105 3.86427505233600

-COOH-Pb²⁺

C -6.38913749000447 0.65946423478089 -0.06163308294748
C -5.82445066545668 1.69428043408262 -0.82007313123948
C -4.44950755858700 1.75977420392335 -0.97343435620049
C -3.62725864020977 0.77198661567896 -0.36565742898662

C	-5.58731794602658	-0.31942635528275	0.55292373964914
C	-4.21481194508655	-0.27123271166237	0.40457257571518
C	-2.22460751194379	0.85841204493266	-0.55858451231937
O	-1.34223777878866	-0.04029971785409	-0.09129387435780
O	-1.62891244568148	1.79028727387078	-1.19735810372955
H	-7.47627625198400	0.61022538575236	0.05657910933836
H	-6.46536932805057	2.44521136876880	-1.28809756248787
H	-3.99359170901702	2.56005522134262	-1.56104464292423
H	-6.04892793363456	-1.11436268265991	1.14329617538700
H	-3.61493454775106	-1.04366236298418	0.89846613554100
Pb	0.53148272777372	1.54449133343547	-1.25763216445524
H	-1.71882097555147	-0.79972428612522	0.39114112401746

-SO₃H-Pb²⁺

C	-6.44198428864289	1.41179210534325	-0.03259641924662
C	-5.84917839421835	1.13485690730898	-1.27070621711352
C	-4.51229779696095	0.75757585058748	-1.33599363412589
C	-3.80439755196125	0.67362689080307	-0.12260108188779
C	-5.71460223370180	1.31606670333241	1.16380936992793
C	-4.37686256316637	0.94726507869385	1.13769304553473
S	-2.15130441052484	0.23858223604992	-0.16016999916331
H	-7.49351406554111	1.71144462694779	0.00337225112242
H	-6.43077637131872	1.22085753118310	-2.19181756551256
H	-4.02906947417083	0.55506415479294	-2.29464004304527
H	-6.19713009569467	1.53181365015089	2.12027825586241
H	-3.80078298171545	0.86751245269256	2.06469844381868
O	-1.64581094347148	-0.00673529268746	-1.55670756537668
O	-1.77093494622660	-1.00551149337373	0.60625100168485
O	-1.31384144786915	1.34504022798456	0.55805002989628
H	-1.57688223357405	2.26548340877127	0.34171894309013
Pb	-0.59567020124128	-2.06709503858091	-1.07099881546578

-NCS-Pb²⁺(S)

H	-2.11567644977099	4.28558565482921	3.65975667114852
C	-2.32977235139145	3.21947416443412	3.55289940889502
C	-2.82621869200235	2.48653342923843	4.63937793281650
H	-2.99586588073825	2.98980400076524	5.59535124779743
C	-3.11311256813148	1.12020429615057	4.52046662689466
H	-3.50393867254450	0.56488907718790	5.37635614084695
C	-2.90599596612560	0.46773541061666	3.31208985262272
H	-3.13188966275648	-0.59508523278304	3.19695926996893
C	-2.40575319409214	1.21981326168193	2.23280919098575
N	-2.21280676277422	0.58929784779415	1.01444826525984
C	-2.11405750803078	2.59303522736309	2.33270186120635
H	-1.73788669886943	3.14887421514906	1.47046591198460
C	-2.06681264286378	0.07294758726276	-0.01294537277461
S	-2.10137490009784	-0.60764488773694	-1.54580752284934
Pb	0.31792195018932	-1.43372405195315	-1.67144948480336

-NCS-Pb²⁺(N)

H	-0.00624279742117	2.37718890853412	3.45340651834117
C	-1.03952513233007	2.05808805273095	3.28540697422142
C	-2.09467263177685	2.84009981461316	3.78520103378625
H	-1.87444588278336	3.76352821005230	4.32744842148226
C	-3.41413061958799	2.45518384550711	3.57349151277578
H	-4.24024379292509	3.08343369519578	3.91902781133037
C	-3.68536565713041	1.26988240670040	2.85349792620758
H	-4.69602424480964	1.09771251588885	2.44792886546117
C	-2.59978268702213	0.48919019802712	2.35851374452576
N	-2.98103715940243	-0.79741201519234	1.84960714210954
C	-1.27698791239524	0.86533443774768	2.59317470065683
H	-0.44678192475597	0.24648595315723	2.24110410473032
C	-2.50612930250188	-1.41847651198836	0.85589203912778
S	-1.98461658954781	-2.19598197185329	-0.33691229190457
Pb	-4.03212366560985	-1.06598753912077	3.90931149714821

-NCO-Pb²⁺(N)

H	-0.91602221285803	3.61104497479492	3.72464919144819
C	-1.64773633525729	2.80665478805912	3.59882701595345
C	-2.54089262751780	2.50093749474472	4.63238399722685
H	-2.50577446171729	3.06773150918090	5.56736482869502
C	-3.47334203839574	1.46834649202910	4.47958191109350
H	-4.16556868026787	1.22745838678827	5.29232551292010
C	-3.53754312104221	0.73630076227703	3.28073866791591
H	-4.29335346867437	-0.04455607849481	3.13558220886359

C	-2.66681915758460	1.08843962602624	2.22380571402815
N	-2.55118547943874	0.18778542583260	1.10104611019252
C	-1.68597379702557	2.09341145044600	2.38769025600017
H	-1.01923020593910	2.35512365475766	1.55785137161924
C	-3.09783936461997	0.21834235611139	-0.02663383135361
O	-3.55377823146028	0.17769116410954	-1.06719785581841
Pb	-1.09419081820107	-0.75214200666272	2.71966490121522

-NCO-Pb²⁺ (O)

H	-1.61595814915216	4.28957061789729	3.49740687543347
C	-2.01501368636481	3.27292946994060	3.52155681197053
C	-2.55908978442319	2.75699822607847	4.70297600641733
H	-2.58565830770094	3.37851276111839	5.60194012964124
C	-3.06917254101428	1.45484728752099	4.74857601040681
H	-3.49088747665399	1.06143859095821	5.67635636086143
C	-3.04298931370167	0.65384837904053	3.61109438910959
H	-3.43817750991954	-0.36420407510792	3.62900191558197
C	-2.49739092369546	1.19358051551445	2.43925965844859
N	-2.47792414174940	0.39840613884409	1.28004882355425
C	-1.97749123965180	2.49248878861686	2.36996380816178
H	-1.55543069920015	2.87938071937834	1.43966103735671
C	-2.47275025136884	-0.25321552548573	0.32935716080983
O	-2.46875011994939	-0.95578391538683	-0.69724921165956
Pb	-2.50173585545433	-2.16735797892776	-2.45123977609404

8) References

- [1] Andersson MP, Stipp SLS. *J. Comput. Chem.*, **2014**, *35*, 2070–5.
- [2] Wander MCF, Clark AE. *Inorg. Chem.*, **2008**, *47*, 8233–41.
- [3] Kuznetsov AM, Masliy AN, Korshin G V. *J. Mol. Model.*, **2018**, *24*, 193–205.
- [4] Dunning TH. *J. Chem. Phys.*, **1989**, *90*, 1007–23.
- [5] Kendall RA, Dunning TH, Harrison RJ. *J. Chem. Phys.*, **1992**, *96*, 6796–806.
- [6] Peterson KA. *J. Chem. Phys.*, **2003**, *119*, 11099–112.
- [7] Metz B, Stoll H, Dolg M. *J. Chem. Phys.*, **2000**, *113*, 2563–9.
- [8] Weigend F, Ahlrichs R. *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297–305.
- [9] Weigend F. *Phys. Chem. Chem. Phys.*, **2006**, *8*, 1057–65.
- [10] Keith JA, Carter EA. *J. Chem. Theory Comput.*, **2012**, *8*, 3187–206.
- [11] Bryantsev VS, Diallo MS, Goddard WA. *J. Phys. Chem. B*, **2008**, *112*, 9709–19.
- [12] Mardirossian N, Head-Gordon M. *Phys. Chem. Chem. Phys.*, **2014**, *16*, 9904–24.
- [13] Najibi A, Goerigk L. *J. Chem. Theory Comput.*, **2018**, *14*, 5725–5738.
- [14] Persson I, Lyczko K, Lundberg D, Eriksson L, Pjaczek A. *Inorg. Chem.*, **2011**, *50*, 1058–72.
- [15] Zhao X, Wang Y, Li Y, Xue W, Li J, Wu H, et al. *J. Chem. Eng. Data*, **2019**, *64*, 2728–35.
- [16] Marcus Y. *J. Chem. Soc. Faraday Trans.*, **1991**, *87*, 2995–9.
- [17] Becke AD. *J. Chem. Phys.*, **1993**, *98*, 5648–52.
- [18] Dunning TH. *J. Chem. Phys.*, **1989**, *90*, 1007–23.
- [19] Cox CS, Cossich Galicia V, Lessio M. *J. Phys. Chem. C*, **2021**, *125*, 3157–68.
- [20] Kesharwani MK, Martin JML. *Theor. Chem. Acc.*, **2014**, *133*, 233–46.
- [21] Minenkov Y, Singstad Å, Occhipinti G, Jensen VR. *Dalt. Trans.*, **2012**, *41*, 5526–41.
- [22] Santra G, Martin JML. *AIP Conf. Proc.*, **2019**, 1–5.