# Role of ligand spacer length of a tripodal amide on uranium(VI) and plutonium(IV) complexation: Synthesis, solvent extraction, liquid membrane transport and theoretical studies

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# Electronic supporting information (ESI)

**CONTENTS**

**S1. EXPERIMENTAL**

**S1.1 Radiotracer purification**

Pu (mainly $^{239}Pu$) purification comprises the addition of a few drops of an aqueous $NaNO_2$ solution for valency adjustment of Pu to the +4 state and subsequent extraction of Pu from 1 M $HNO_3$ solution using a 0.5 M TTA solution in xylene. The extracted Pu was stripped back to the aqueous phase using 8 M $HNO_3$ and its radionuclidic purity was checked by alpha spectrometry.

$^{233}U$ was purified using a DOWEX 1x8 (chloride form, 100-200 mesh) anion exchange resin column for the separation of its daughter products as reported before. [1]$^{241}Am$ taken from the laboratory stock was purified from its daughter product $^{237}Np$ using an anion exchange resin column. The radionuclide purity of these radiotracers was checked and confirmed by alpha and gamma ray spectrometry.

**S1.2 Liquid-liquid extraction**

The liquid-liquid extraction studies were carried out by taking equal volumes (1.0 mL) of the aqueous (consisting of the radiotracer spiked in dilute nitric acid solution) and the organic phases containing the ligand solution in leak tight Pyrex glass tubes and equilibrating in a constant temperature (25 ± 1 °C) water bath for about 1 hour which was optimized by a set of experiments (*vide infra*). The organic phase containing the ligand solution was in 90% *n*-dodecane + 10% isodecanol or *n*-dodecane depending on the ligand solubility. After equilibration, the tubes were centrifuged at 1700 RCF for 5 minutes and a suitable quantity (usually 100 µL) of the solution from the organic and the aqueous phases were removed and assayed by radiometry. While $^{233}U$ and Pu were assayed using liquid scintillation counting using a scintillator cocktail (Perkin Elmer), $^{241}Am$ and $^{252,254}Eu$ were assayed by a NaI(Tl) detector (Para Electronics) coupled to a multi-channel analyzer (ECIL, India). The distribution ratio ($D_M$, where 'M' is the metal ion) was calculated using the following formula:

$$D_M = \frac{Counts\ per\ minute\ per\ mL\ of\ the\ organic\ phase}{Counts\ per\ minute\ per\ mL\ of\ the\ aqueous\ phase} \quad (1)$$

The percentage extraction (%*E*) and the stripping percentage (%*S*) of a metal ion for a phase volume ratio of 1 (ratio of the aqueous phase to organic volume) were measured using the following formula:

$$\%E = \frac{100D_M}{D_M + 1} \quad (2)$$

$$\%S = 100 - \%E \quad (3)$$

The mass balance, the difference between the sum of the final activities in both phases (organic and aqueous) and the total initial activity in the aqueous phase, was found to be within ± 2%.

The distribution ratio of the metal ion ($D_M$) and the extraction equilibrium constant ($K_{ex}$) in a two-phase equilibrium system is defined as follows:

$$D_M = \frac{[M(NO_3)_n \bullet yL]_{org}}{[M^{n+}]_{aq}} \quad (4)$$

$$K_{ex} = \frac{a_{M(NO_3)_n}.yL_{org}}{a_{M^{n+}_{aq}}.a^n_{NO_{3,aq}}.a^y_{L_{free,org}}} \quad (5)$$

where 'a' is the activity of the species and a = γ.c, where 'γ' is the activity coefficient of the respective species and 'c' is the concentration of the species in the solution. Eqn (6) is obtained after considering the activity coefficients of the metal-ligand complex, free ligand and the metal ion tracer as unity.

$$K_{ex} = \frac{[M(NO_3)_n . yL]_{org}}{[M_{aq}^{n+}]_{aq} \, [NO_3]_{aq}^{n} \, [L]_{free,org}^{y} \times \gamma_{NO_{3,aq}}^{n}} \quad (6)$$

Taking the logarithm on both sides of eqn(6), gives the following equation (eqn 7) and using eqn(4):

$$\text{Log } D_M = \text{Log } K_{ex} + \text{n log } [NO_3^-]_{aq} + \text{y log } [L]_{org} + \text{n log } [NO_3^-]_{aq} \quad (7)$$

**S.1.3 Transport studies**

The SLM transport studies were performed in a two-compartment glass cell with 30 mL capacity with provision for taking out samples from each compartment through the sampling ports provided at the top of the cell.
The percentage transport was calculated using the following formula:

$$\% \text{ T} = 100 \times C_{r,t}/C_0 \quad (8)$$

$$\% \text{ R} = 100 \times (C_{f,o}-C_{f,t})/C_o \quad (9)$$

where $C_{f,0}$ is the initial ($t$ = 0) concentration of the radionuclide at the feed phase whereas $C_{f,t}$ and $C_{r,t}$ are the radionuclide concentrations in the feed and the receiver phases, respectively, at time $t$. The permeability coefficient ($P$) was determined using the following equation:

$$\ln \left(\frac{C_{f,t}}{C_{f,0}}\right) = -\left(\frac{Q}{V_f}\right) . P . t \quad (10)$$

where '$Q$' represents effective surface area (4.79 $cm^2$) that was obtained by multiplying the total exposed surface area of the membrane to the porosity of the membrane, '$V_f$' is volume of the feed solution (30 mL).

The SLM transport cell arrangement is presented in Fig. S1. The PTFE flat sheet membrane was kept in the ligand solution (in the diluent mixture comprising of 90% *n*-dodecane + 10% isodecanol) in a covered Petri dish for overnight to soak completely. Prior to use, the membrane was wiped carefully using a small piece of tissue paper to remove the excess ligand solution sticking to the membrane.

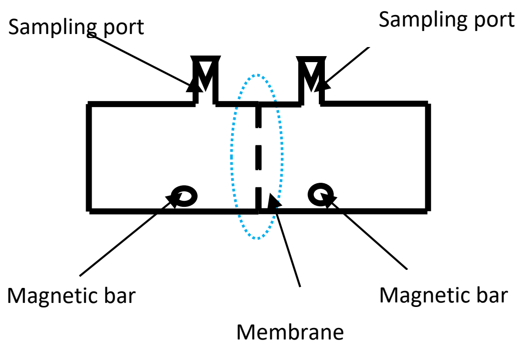



**Fig. S1.** Schematic presentation of SLM transport set up.

The membrane was then kept in between the glass flanges of the two compartments and fixed tightly using Para film to avoid any leakage. Clamp was used to hold the transport cell and to put the set up on a magnetic stirrer. The feed and the strip solutions were filled in the respective compartments and the solutions were stirred using magnetic bars at 200 rpm speed which was optimized in a previous study.[2] Samples were taken out from both the compartments (usually 100 µL aliquots) at regular intervals and the amount of the actinide ion was assayed radiometrically.

### S1.4 Computational studies

The dielectric constant of water and organic solvent (90% dodecane + 10% isodecanol) was taken to be 80 and 3.03, respectively. The Gibbs free energy of complexation for the various complexation reactions has been evaluated using the prescription published earlier.[3]

The model complexation reaction was used as follows:

$$[Pu(H_2O)_{10}]^{4+}_{(aq)} + 4NO_3^-{}_{(aq)} + nL_{(org)} \rightarrow [Pu(NO_3)_4\text{-}L_n]_{(org)} + 10H_2O_{(aq.)} \quad (11)$$

$$[UO_2(H_2O)_5]^{2+}_{(aq)} + 2NO_3^-{}_{(aq)} + nL_{(org)} \rightarrow [UO_2(NO_3)_2\text{-}L_n]_{(org)} + 5H_2O_{(aq.)} \quad (12)$$

Here L stands for HONTA and HONTP. A scalar relativistic effect for heavier actinide elements was included in the present computation using the earlier reported procedure.[4] Since there is a very small effect on the solvation energy between the gas phase and the solvent phase geometry,[5] the aqueous solvent effect was integrated by performing single point energy calculations using the optimized geometry obtained from the B3LYP level of theory employing the COSMO solvation model.

## S2. Results

### S2.1 Solvent extraction studies

#### S2.1.1 Kinetics of extraction and stripping

For U(VI), the extraction was studied at two acidities, *viz*., 0.01 M and 0.001 M $HNO_3$ and in both cases, the metal ion extraction equilibrium was reached within 10 minutes (Fig.S2a). At pH3 (maintained using 0.01 M 1,4-piperazinediethanesulfonic acid (PIPES) buffer solution) the slightly higher *D*-value of U(VI) indicates more availability of free ligands compared to that at pH2. Am(III) yielded a very low *D*-value at 0.001 M $HNO_3$ (Fig.S2a). Similarly, Pu(IV) extraction kinetics was studied at 3 M $HNO_3$, indicating that the equilibrium *D*-value was attained within 10 minutes (Fig.S2b). From the figures it is clear that the extraction kinetics using 0.08 M HONTP was fast for these metal ions.

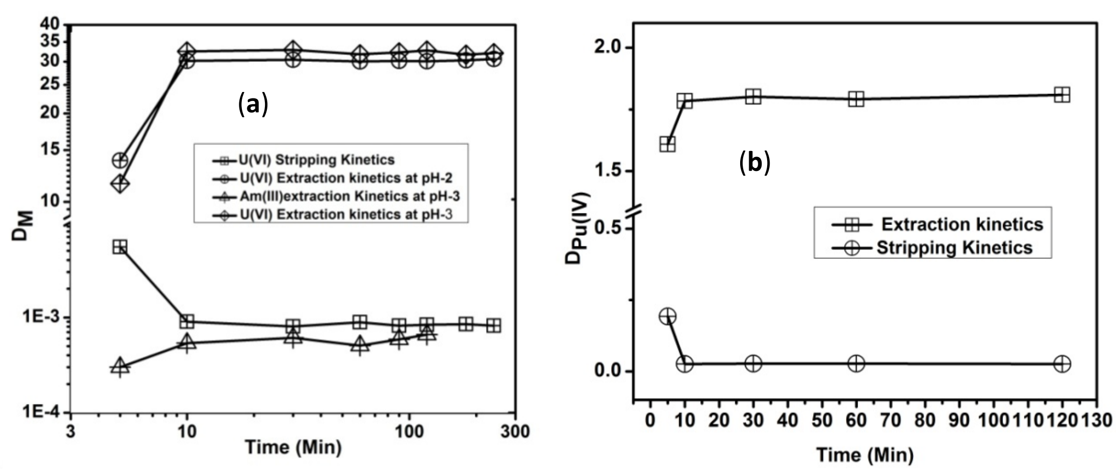



**Fig. S2.** Kinetics of extraction and stripping of Pu(IV), Am(III), and U(VI); Organic phase: 0.08 M HONTPin 90% *n*-dodecane + 10% isodecanol.

#### S2.1.2 Influence of temperature on metal ion extraction

The influence of temperature on the extraction of U(VI) and Pu(IV) was investigated at different temperatures in the range 15°C to 45°C. Extraction of U(VI) was carried out using 0.08 M HONTP in *n*-dodecane (in Fig. S3 mentioned as U-DD) and 0.08 M HONTP in 90% *n*-dodecane + 10% isodecanol (denoted as U-(DD+ID)). A similar study was done for Pu(IV) using 0.08 M HONTP in 90% *n*-dodecane + 10% isodecanol (mentioned as Pu(IV)). The *D*-values of U(VI) decreased with increasing temperature and the extent of the decrease was more in 90% *n*-dodecane + 10% isodecanol medium than in *n*-dodecane. For Pu(IV), on the other hand, a slight increase in the *D*-values was observed with increasing temperature. This is in line as reported for the extraction of these metal ions with neutral donor ligands such as TBP.[6] The straight-line plots of log $D_M$*vs*. 1/T are presented in Fig. S3 giving slope values of 2953 ± 254 and 6608.6 ± 40.8 for U(VI) forthe organic phases containing *n*-dodecane and 90% *n*-dodecane + 10% isodecanol, respectively. Similarly for Pu(IV), the slope value was -387 ± 26 using 0.08 M HONTP in 90% *n*-dodecane + 10% isodecanol.
The enthalpy changes of the reaction, Δ*H*, were determined using eqn (13). Where *R* is the universal gas constant (8.314 J $mol^{-1}K^{-1}$).

$$\frac{\Delta \log D_M}{\Delta(\frac{1}{T})} = \frac{-\Delta H}{2.303R} \tag{13}$$

The values of Δ*H* for the processes were calculated to be -56.5 ± 4.8 kJ $mol^{-1}$, -126.5 ± 0.7 kJ $mol^{-1}$ and 7.4 ± 0.5 kJ $mol^{-1}$ for U(VI) extraction using HONTP in *n*-dodecane, U(VI) and Pu(IV) extraction by the ligand in 90% *n*-dodecane + 10% isodecanol, respectively. This indicates that the extraction of U(VI) is exothermic, whereas the extraction of Pu(IV) is endothermic. Eqn (6) can be expressed as

$$K_{ex} = \frac{D_M(1 + \sum \beta_p^M [NO_3^-]^p)}{[NO_3]_{aq}^4 L_{free,org} \times \gamma_{NO_{3,aq}}^4} \tag{14}$$

where $\beta_p^M$ is the overall stability constant for the complexes of Pu(IV) and U(VI) of the types of $Pu(NO_3)_p^{4-p}$ and $UO_2(NO_3)_p^{2-p}$. $K_{ex}$ is the extraction constant. Assuming $L_{free}$ as the initial ligand concentration (tracer metal ion concentration is used), we can determine $K_{ex}$ values at a given nitrate and ligand concentration. The mean ionic activity coefficient of nitrate at 3 M $HNO_3$ was 1.15 and at 0.01 M $HNO_3$ was 0.906.[7] The nitrate concentration in the aqueous phase was determined considering the dissociation constant of $HNO_3$ ($K_{HNO3}$: 23.5).[8] The value of (1+ $\beta_p^M [NO_3^-]^p$) at 0.01 M $HNO_3$ was taken as 1.0 for U(VI), and that for Pu(IV) was taken as 105 at 3 M $HNO_3$ from refs. 9 and 10. The free energy change Δ*G* can be expressed as

$$\Delta G = -RT ln K_{ex} \tag{15}$$

The entropy change of a reaction is represented in terms of Δ*H* and Δ*G*as follows:

$$\Delta S = \frac{\Delta H}{T} - \frac{\Delta G}{T} \tag{16}$$

*R* is the molar gas constant (8.314 J $mol^{-1}$ $K^{-1}$). Different values of the extraction constant ($K_{ex}$) were evaluated using eqn (6) at 0.08 M ligand and taking nitrate ion concentrations of 0.01 M and 2.7 M for U(VI) and Pu(IV), respectively (considering $K_{HNO3}$). $D_{U(VI)}$ decreases with the increase of temperature, whereas $D_{Pu(IV)}$ slightly increases with the increase of temperature suggesting the former process is exothermic in nature, whereas the latter process is endothermic in nature (Fig. S3). The free energy change (Δ*G*) was calculated considering a temperature of 25°C using eqn (7). The free energy changes obtained for the two-phase extraction processes are -28.8, -44.2, and -5.15 kJ $mol^{-1}$ for U(VI) extraction using the ligand in *n*-dodecane, and those of U(VI) and Pu(IV) extraction by HONTP in 90% *n*-dodecane + 10% isodecanol, respectively, while the entropy changes for the processes are -0.09, -0.28, and 0.04 kJ $mol^{-1}$ $K^{-1}$,respectively.

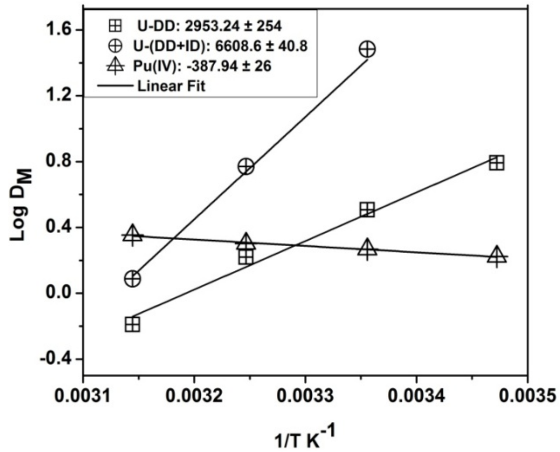
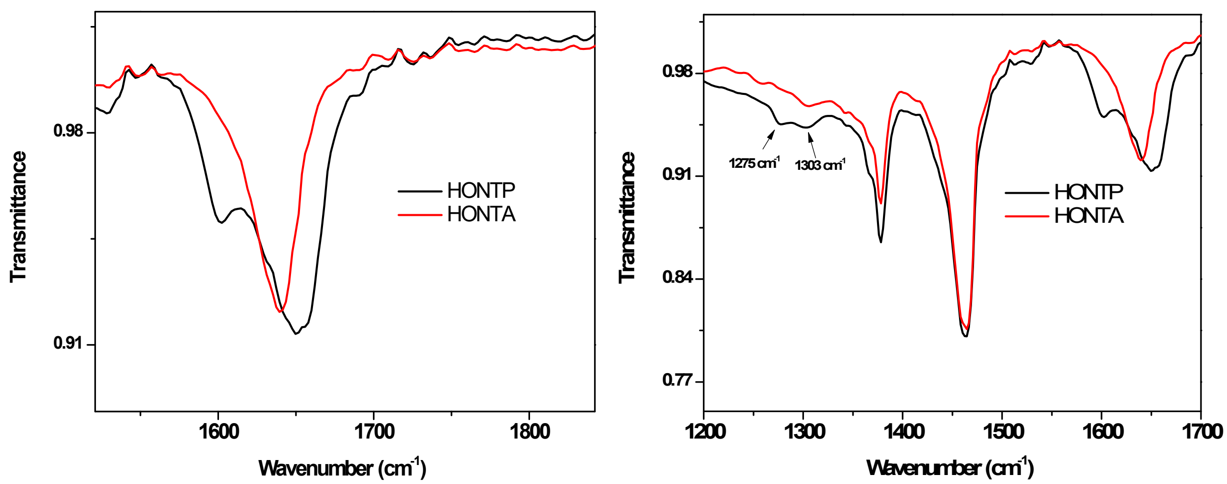



**Fig. S3.** Dependence of log $D_M$ values on the temperature. Aqueous phase: 3 M $HNO_3$ and 0.01 M $HNO_3$ for Pu(IV) and U(VI), respectively; Organic phase:0.08 M ligand in 90% *n*-dodecane + 10% isodecanol or 0.08 M ligand in *n*-dodecane.

### S2.1.3 ATR-FTIR studies

ATR-FTIR studies of the extracted samples were carried out using an ALPHA II, Bruker ATR-FTIR instrument. The spectra of the extracted samples are shown below.




(a) (b)

**Fig. S4.** ATR-FTIR spectra (a) (1520-1840 $cm^{-1}$ region) (b) (1200-1700 $cm^{-1}$ region) of the extract of U(VI) at pH 2.0 with 0.08 M HONTA/HONTP in 90% *n*-dodecane + 10% isodecanol.

## S2.2 SLM studies

### S2.2.1 Stability of membrane

For any practical application of any SLM transport system, the long-term stability of the membrane should be good. Many factors are responsible for the stability of a membrane[11] such as trans-membrane pressure, leaching of extractant solution from the membrane to adjacent aqueous phases, wetting of membrane pores by aqueous solution, resulting water channel formation, blockage of membrane pores due to emulsion formation and solid particles, etc. Diluents also play important roles for the stability of liquid membranes, e.g., the stability of a liquid membrane using non-polar diluents (*e.g.*, *n*-dodecane) is better than with polar diluents (e.g., nitrobenzene, chloroform).[12,13] Our previous studies have shown a good stability of a SLM containing a mixture of *n*-dodecane + isodecanol as the diluent.[14] In the present work, the same SLM was used for the stability study, while replacing the feed and strip solutions with fresh solutions each time.

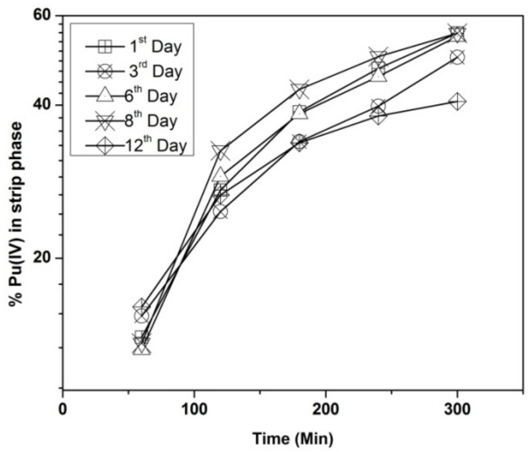



**Fig. S5.** Transport of Pu(IV) across a flat PTFE sheet SLM; Feed phase: 3 M $HNO_3$; Strip phase: 0.5 M oxalic acid + 0.5 M $HNO_3$; Carrier ligand: 0.08 M HONTP in 90% *n*-dodecane + 10% isodecanol.

The transport efficiency was tested for five different cycles over a period of 12 days. Fig. S5 suggests that the membrane has a reasonably good stability up to 8 days. The % transport and permeability coefficient (*P*) values are calculated and presented in Table S1. The *P* values are nearly constant till the 8th day.

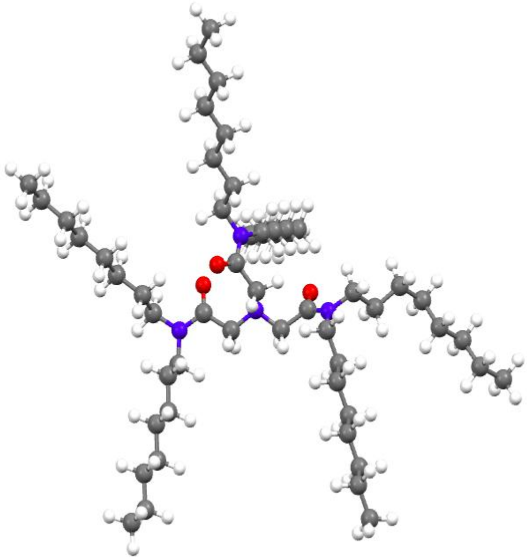
**Table S1**Continuous transport of Pu(IV) using the same membrane phase (0.08 M HONTP in 90% *n*-dodecane + 10% isodecanol) and fresh feed (3 M $HNO_3$) and strip (0.5 M $HNO_3$ + 0.5 M oxalic acid) solutions over 12 days. Feed and strip volumes: 30 mL; Transport data at 5 h

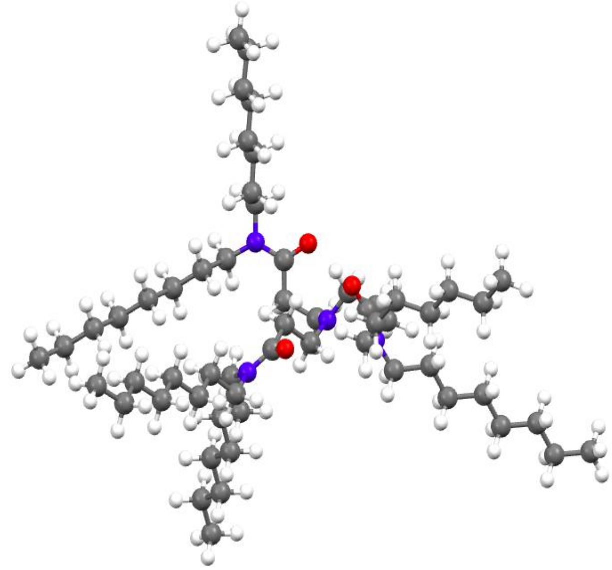
| Day | % Transport | $P_{Pu(IV)} \times 10^3$ (cm $s^{-1}$) |
|---|---|---|
| 1 | 55.45 | 0.38 ± 0.01 |
| 3 | 49.69 | 0.28 ± 0.02 |
| 6 | 54.62 | 0.29 ± 0.02 |
| 8 | 55.39 | 0.31 ± 0.01 |
| 12 | 40.70 | 0.17 ± 0.02 |

**S2.3 Computational studies**

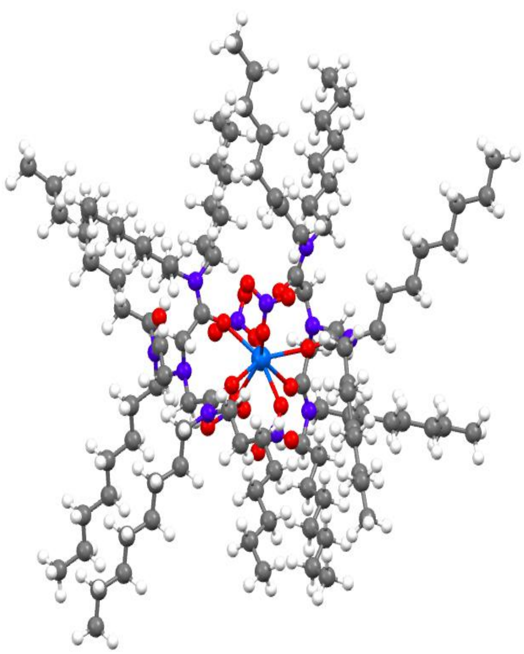
**Table S2** Calculated value of complexation free energy (kcal/mol) in the solution phase

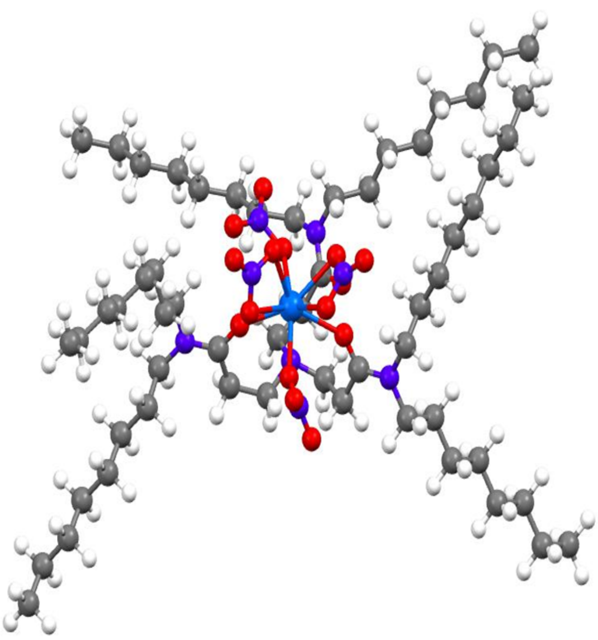
| Reaction | Solution phase complexation free energy | Partial NPA charge on Pu/U atom |
|---|---|---|
| $[Pu(H_2O)_{10}]^{+4}$ + $4NO_3^-$ + 2HONTA = $Pu(NO_3)_4$-$(HONTA)_2$+ $10H_2O$ | -57.9 | 1.889 |
| $[Pu(H_2O)_{10}]^{+4}$ + $4NO_3^-$ + HONTP = $Pu(NO_3)_4$-(HONTP)+ $10H_2O$ | -85.5 | 1.623 |
| $[UO_2(H_2O)_5]^{+2}$+ $2NO_3^-$ + HONTA = $UO_2(NO_3)_2$-HONTA+ $5H_2O$ | -26.9 | 1.931 |
| $[UO_2(H_2O)_5]^{+2}$+ $2NO_3^-$ + 2HONTP = $UO_2(NO_3)_2$-$(HONTP)_2$+ $5H_2O$ | 6.5 | 1.858 |



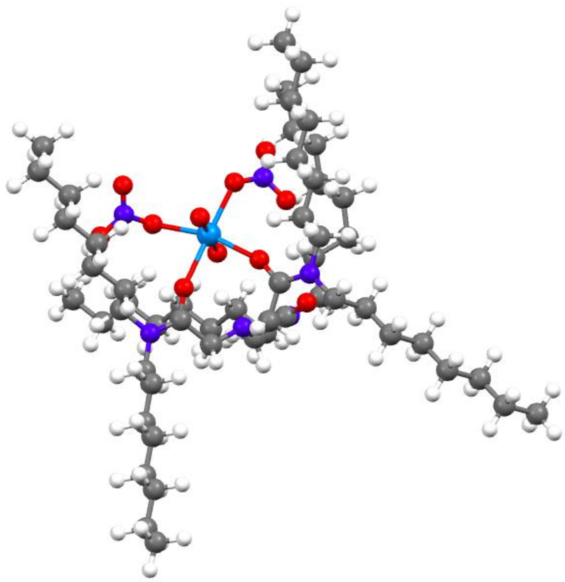


**(a)** **(b)**

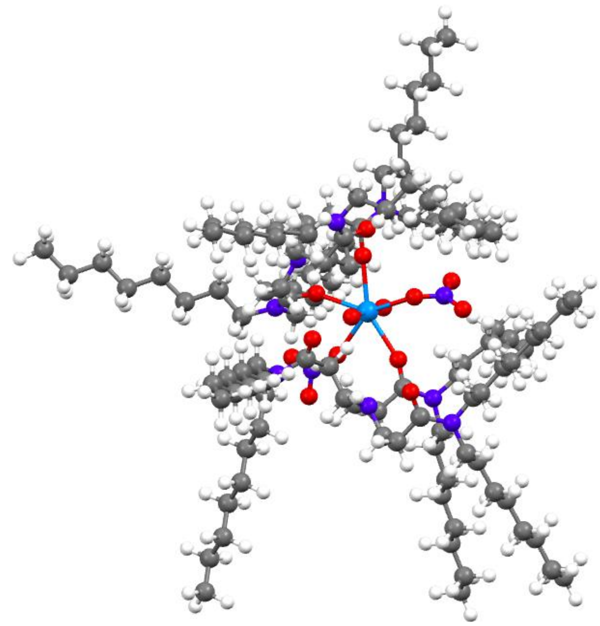




**(c)** **(d)**



**(e)**



**(f)**

**Fig. S6:** Optimized structure of (a) HONTA; (b) HONTP; (c) $Pu^{4+}$ - HONTA; (d) $Pu^{4+}$ - HONTP; (e) $UO_2^{2+}$ - HONTA and (f) $UO_2^{2+}$ - HONTP. The grey and white spheres correspond to C and H atoms, whereas red and blue ones denote O and N atoms and cyan spheres represent Pu or U atoms.

### S2.3.1 Optimized coordinates

HONTA

| | | | |
|---|---|---|---|
| N | -0.3486093 | 0.5711933 | -0.7397415 |
| C | -0.4942358 | 1.9669532 | -1.1213231 |
| H | -0.9559332 | 2.5009946 | -0.2737746 |
| H | 0.4981141 | 2.4458235 | -1.2854014 |
| C | 0.5106188 | -0.1983591 | -1.6407635 |
| H | 0.7742903 | -1.1399592 | -1.1356982 |
| H | 1.4599062 | 0.3386675 | -1.8505207 |
| C | 0.1159696 | 0.4960844 | 0.6454009 |
| H | -0.5856247 | 1.0729998 | 1.2679545 |
| H | 1.1145737 | 0.9646899 | 0.7738856 |
| C | -1.3865659 | 2.2183137 | -2.3480202 |
| C | -0.0274197 | -0.5558571 | -3.0412748 |
| C | 0.0546700 | -0.9263651 | 1.2277715 |
| O | -1.0346372 | -1.4659247 | 1.3712187 |
| O | -2.0730708 | 1.3326425 | -2.8313138 |
| O | 0.5025289 | -0.0360102 | -4.0193685 |
| N | -0.9834348 | -1.5234118 | -3.1563925 |
| N | 1.2164602 | -1.5594180 | 1.6010601 |
| N | -1.3871502 | 3.4896268 | -2.8687722 |
| C | -1.3904827 | -1.9009355 | -4.5093564 |
| C | -0.5606898 | -3.0563067 | -5.0833109 |
| H | -1.2920289 | -1.0171485 | -5.1548717 |
| H | -2.4567337 | -2.1775674 | -4.4846284 |
| C | -0.9964783 | -3.4703823 | -6.4915659 |
| H | 0.4993710 | -2.7503018 | -5.0971266 |
| H | -0.6294352 | -3.9275311 | -4.4056538 |
| C | -0.2350513 | -4.6824417 | -7.0377800 |
| H | -2.0804049 | -3.6942539 | -6.4911092 |
| H | -0.8677830 | -2.6144358 | -7.1799886 |
| H | 0.8512374 | -4.4757974 | -7.0075362 |
| H | -0.3935946 | -5.5428549 | -6.3604474 |
| C | -1.7007467 | -2.1487160 | -2.0457111 |
| C | -3.1072526 | -1.5921168 | -1.7889169 |
| H | -1.1165283 | -2.0451328 | -1.1247372 |
| H | -1.7607228 | -3.2337548 | -2.2526975 |
| C | -3.8090586 | -2.3009830 | -0.6271532 |
| H | -3.0126893 | -0.5161041 | -1.5845426 |
| H | -3.7185171 | -1.6818401 | -2.7053595 |
| C | -5.2138860 | -1.7583909 | -0.3466661 |
| H | -3.8751145 | -3.3872518 | -0.8345701 |
| H | -3.1884214 | -2.1952516 | 0.2789416 |
| H | -5.1447905 | -0.6742488 | -0.1385892 |
| H | -5.8344779 | -1.8472572 | -1.2585847 |
| C | -2.1768047 | 3.6992450 | -4.0876470 |
| C | -1.4561478 | 3.2834128 | -5.3768058 |
| H | -2.4535792 | 4.7661479 | -4.1286598 |
| H | -3.1061002 | 3.1168705 | -3.9928285 |
| C | -2.3516000 | 3.4006362 | -6.6133466 |

| | | | |
|---|---|---|---|
| H | -0.5535811 | 3.9051080 | -5.5125263 |
| C | -1.6322423 | 3.0675827 | -7.9241794 |
| H | -3.2244460 | 2.7318939 | -6.4946379 |
| H | -2.7658862 | 4.4256057 | -6.6777194 |
| H | -0.7763490 | 3.7568082 | -8.0531815 |
| H | -1.1912945 | 2.0563992 | -7.8500590 |
| C | -0.7478956 | 4.6460802 | -2.2501910 |
| C | 0.5161582 | 5.1636389 | -2.9519118 |
| H | -0.5091132 | 4.4145746 | -1.2030782 |
| H | -1.4922875 | 5.4629697 | -2.2063693 |
| C | 1.1460984 | 6.3423556 | -2.2030862 |
| H | 1.2432638 | 4.3379455 | -3.0495456 |
| H | 0.2637472 | 5.4713389 | -3.9813730 |
| C | 2.3430779 | 6.9777575 | -2.9177348 |
| H | 0.3763030 | 7.1187986 | -2.0337136 |
| H | 1.4580659 | 6.0097429 | -1.1948374 |
| H | 3.1113520 | 6.2057618 | -3.1092138 |
| H | 2.0225985 | 7.3347061 | -3.9143266 |
| C | 2.5675921 | -1.0179846 | 1.4428347 |
| C | 3.1015716 | -0.2261046 | 2.6438218 |
| H | 2.6108378 | -0.3929028 | 0.5393471 |
| H | 3.2389369 | -1.8696966 | 1.2425007 |
| C | 4.5295021 | 0.2832949 | 2.4270460 |
| H | 2.4258517 | 0.6245871 | 2.8457703 |
| H | 3.0671502 | -0.8609323 | 3.5459628 |
| C | 5.0882361 | 1.0757738 | 3.6128678 |
| H | 5.1953713 | -0.5746482 | 2.2160685 |
| H | 4.5608958 | 0.9140364 | 1.5186293 |
| H | 4.4281261 | 1.9395364 | 3.8175512 |
| H | 5.0471675 | 0.4473690 | 4.5222927 |
| C | 1.0671695 | -2.8958560 | 2.1941927 |
| C | 0.7170730 | -2.9041452 | 3.6877557 |
| H | 2.0085720 | -3.4427207 | 2.0244325 |
| H | 0.2716804 | -3.4180010 | 1.6416115 |
| C | 0.4828930 | -4.3244500 | 4.2157163 |
| H | 1.5228708 | -2.4110525 | 4.2572258 |
| H | -0.1956907 | -2.3037482 | 3.8357553 |
| C | 0.1575800 | -4.4115311 | 5.7140853 |
| H | -0.3468312 | -4.7766768 | 3.6437836 |
| H | 1.3709591 | -4.9502946 | 4.0026404 |
| H | -0.1890772 | -5.4360875 | 5.9402483 |
| H | -0.6988290 | -3.7490935 | 5.9399445 |
| H | -1.1031581 | 2.2450425 | -5.2635721 |
| C | -0.6334464 | -5.0818856 | -8.4619408 |
| C | 0.0803830 | -6.3368276 | -8.9742672 |
| H | -0.4302479 | -4.2386319 | -9.1486618 |
| H | -1.7273524 | -5.2433701 | -8.5032253 |
| H | 1.1750964 | -6.1863720 | -8.9136451 |
| H | -0.1415242 | -7.1826519 | -8.2960254 |
| C | -0.2945879 | -6.7290830 | -10.4072343 |
| C | 0.3989334 | -8.0030586 | -10.8938174 |
| H | -0.0512261 | -5.8927782 | -11.0884851 |

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| H | -1.3908460 | -6.8581250 | -10.4729932 |
| H | 0.1119079 | -8.2528890 | -11.9282445 |
| H | 1.4970395 | -7.8967701 | -10.8700493 |
| H | 0.1396617 | -8.8673200 | -10.2587548 |
| C | -2.5305241 | 3.1400275 | -9.1627329 |
| C | -1.7964615 | 2.8553075 | -10.4766859 |
| H | -2.9991323 | 4.1411456 | -9.2170568 |
| H | -3.3670975 | 2.4250396 | -9.0489215 |
| H | -0.9724923 | 3.5840813 | -10.5982394 |
| H | -1.3096580 | 1.8634781 | -10.4160088 |
| C | -2.6947714 | 2.8996048 | -11.7170145 |
| C | -1.9449746 | 2.6379519 | -13.0246304 |
| H | -3.1943141 | 3.8848235 | -11.7689919 |
| H | -3.5077404 | 2.1588179 | -11.6030660 |
| H | -2.6200686 | 2.6731204 | -13.8952285 |
| H | -1.1521842 | 3.3877639 | -13.1885384 |
| H | -1.4620719 | 1.6458136 | -13.0183866 |
| C | 2.9688163 | 8.1393406 | -2.1386792 |
| C | 4.1265990 | 8.8319986 | -2.8635816 |
| H | 3.3211701 | 7.7706784 | -1.1568003 |
| H | 2.1855138 | 8.8869071 | -1.9119989 |
| H | 4.9090925 | 8.0875465 | -3.1032245 |
| H | 3.7694428 | 9.2143104 | -3.8384986 |
| C | 4.7506788 | 9.9836777 | -2.0678173 |
| C | 5.8861596 | 10.6964625 | -2.8042027 |
| H | 5.1233409 | 9.5960790 | -1.1016087 |
| H | 3.9619633 | 10.7149631 | -1.8115852 |
| H | 6.3103714 | 11.5148452 | -2.1999546 |
| H | 6.7078361 | 10.0008286 | -3.0453047 |
| H | 5.5356806 | 11.1325823 | -3.7551492 |
| C | 6.5224376 | 1.5718613 | 3.4050335 |
| C | 7.0812897 | 2.3659145 | 4.5892872 |
| H | 6.5636204 | 2.1976244 | 2.4935867 |
| H | 7.1814846 | 0.7066921 | 3.2021551 |
| H | 6.4233540 | 3.2325077 | 4.7911013 |
| H | 7.0380069 | 1.7408156 | 5.5013128 |
| C | 8.5171316 | 2.8601146 | 4.3846976 |
| C | 9.0658093 | 3.6546325 | 5.5708562 |
| H | 8.5597107 | 3.4826348 | 3.4719198 |
| H | 9.1741690 | 1.9934460 | 4.1852171 |
| H | 10.0982539 | 3.9943032 | 5.3888293 |
| H | 8.4523294 | 4.5492905 | 5.7728367 |
| H | 9.0732404 | 3.0472080 | 6.4919490 |
| C | 1.3240976 | -4.0747545 | 6.6504314 |
| C | 0.9861277 | -4.2321036 | 8.1362492 |
| H | 1.6687942 | -3.0400516 | 6.4705524 |
| H | 2.1842027 | -4.7256011 | 6.4020949 |
| H | 0.1324611 | -3.5748957 | 8.3886234 |
| H | 0.6329699 | -5.2640977 | 8.3226755 |
| C | 2.1563468 | -3.9230206 | 9.0754984 |
| C | 1.8137474 | -4.0853857 | 10.5574249 |
| H | 2.5090139 | -2.8914713 | 8.8894117 |

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| H | 3.0082266 | -4.5802148 | 8.8201706 |
| H | 2.6796541 | -3.8605935 | 11.2012057 |
| H | 0.9932566 | -3.4109594 | 10.8564614 |
| H | 1.4904473 | -5.1157710 | 10.7836656 |
| C | -5.9266816 | -2.4510408 | 0.8186702 |
| C | -7.3162356 | -1.8832524 | 1.1233371 |
| H | -5.2962208 | -2.3780199 | 1.7244291 |
| H | -6.0142301 | -3.5330731 | 0.6031205 |
| H | -7.2274062 | -0.8018570 | 1.3412734 |
| H | -7.9473286 | -1.9526443 | 0.2170063 |
| C | -8.0321241 | -2.5735005 | 2.2887920 |
| C | -9.4122526 | -1.9884057 | 2.5942331 |
| H | -7.3972660 | -2.5111868 | 3.1918584 |
| H | -8.1298810 | -3.6525758 | 2.0674071 |
| H | -9.8977676 | -2.5079959 | 3.4364632 |
| H | -9.3446683 | -0.9189770 | 2.8578205 |
| H | -10.0839906 | -2.0687177 | 1.7224387 |

HONTA-C2

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| N | 2.3620734 | 1.8505010 | 0.4009829 |
| H | 2.5111420 | 3.8349145 | 0.9679008 |
| H | 3.9437766 | 3.1857059 | 0.1580493 |
| C | 2.8795472 | 0.7584728 | -0.3895359 |
| H | 3.0145004 | -0.1351207 | 0.2478425 |
| H | 3.8914371 | 1.0382812 | -0.7301044 |
| C | 1.1368542 | 1.6547674 | 1.1646001 |
| H | 0.2532860 | 1.4501672 | 0.5334868 |
| H | 0.9205678 | 2.6033874 | 1.6708653 |
| C | 0.9548804 | 4.2426541 | -1.2912495 |
| C | 2.5346139 | -0.9946221 | -2.2252498 |
| C | 0.8772203 | -0.8443623 | 1.6542364 |
| O | -0.1090573 | -0.9526018 | 0.9336837 |
| O | 0.1938523 | 4.0659642 | -0.3485498 |
| O | 2.0906587 | -2.0715496 | -1.8426337 |
| N | 3.5119663 | -0.9541784 | -3.2006932 |
| N | 1.6447881 | -1.9394211 | 1.9740846 |
| N | 0.5004806 | 4.7758507 | -2.4766667 |
| C | 3.8992439 | -2.2319007 | -3.8050803 |
| C | 3.0145263 | -2.6339395 | -4.9913205 |
| H | 3.8386214 | -3.0051132 | -3.0260641 |
| H | 4.9513999 | -2.1620088 | -4.1263310 |
| C | 3.4108198 | -3.9815195 | -5.6009074 |
| H | 1.9688010 | -2.6774550 | -4.6435440 |
| H | 3.0576970 | -1.8480876 | -5.7687494 |
| C | 2.5834025 | -4.3675248 | -6.8309945 |
| H | 4.4828583 | -3.9634695 | -5.8761356 |
| H | 3.3123107 | -4.7694069 | -4.8309482 |
| H | 1.5091854 | -4.3442217 | -6.5691250 |
| H | 2.7167127 | -3.5973175 | -7.6144065 |
| C | 4.1748090 | 0.2427292 | -3.7015610 |

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| C | 5.6108704 | 0.4301391 | -3.1870994 |
| H | 3.5761544 | 1.1265735 | -3.4435700 |
| H | 4.1883915 | 0.2025938 | -4.8068419 |
| C | 6.3181631 | 1.6488203 | -3.7864450 |
| H | 5.5904696 | 0.5115503 | -2.0863485 |
| H | 6.2003498 | -0.4763480 | -3.4101278 |
| C | 7.7508689 | 1.8300661 | -3.2749617 |
| H | 6.3315084 | 1.5598187 | -4.8890641 |
| H | 5.7334346 | 2.5625160 | -3.5678975 |
| H | 7.7325769 | 1.9289991 | -2.1734756 |
| H | 8.3265563 | 0.9082545 | -3.4801904 |
| C | -0.9340835 | 5.0709578 | -2.5642822 |
| C | -1.8065004 | 3.8627059 | -2.9268825 |
| H | -1.0670426 | 5.8739213 | -3.3085369 |
| H | -1.2567702 | 5.4617073 | -1.5872941 |
| C | -3.3027465 | 4.1886479 | -2.9341344 |
| H | -1.5079631 | 3.4735507 | -3.9164509 |
| C | -4.1774369 | 3.0166381 | -3.3906141 |
| H | -3.6107981 | 4.5050125 | -1.9204311 |
| H | -3.4912641 | 5.0594505 | -3.5914602 |
| H | -3.8913547 | 2.7329147 | -4.4210911 |
| H | -3.9553222 | 2.1319653 | -2.7655237 |
| C | 1.3563445 | 5.1116221 | -3.6096904 |
| C | 1.4287693 | 4.0648238 | -4.7318534 |
| H | 2.3728579 | 5.3222531 | -3.2470240 |
| H | 0.9914989 | 6.0636203 | -4.0336393 |
| C | 2.3668439 | 4.4935781 | -5.8633483 |
| H | 1.7636030 | 3.1005492 | -4.3097610 |
| H | 0.4173339 | 3.8845709 | -5.1347205 |
| C | 2.4676090 | 3.4871076 | -7.0140458 |
| H | 2.0314104 | 5.4687882 | -6.2637668 |
| H | 3.3775725 | 4.6746607 | -5.4505123 |
| H | 2.8118169 | 2.5130241 | -6.6186250 |
| H | 1.4588414 | 3.3017997 | -7.4277539 |
| C | 2.8142867 | -1.9091012 | 2.8477570 |
| C | 2.5217829 | -2.0304851 | 4.3508299 |
| H | 3.3932600 | -0.9902585 | 2.6650834 |
| H | 3.4731958 | -2.7373597 | 2.5402448 |
| C | 3.7937041 | -1.9614623 | 5.2012785 |
| H | 1.8284743 | -1.2249106 | 4.6506989 |
| H | 1.9902724 | -2.9785437 | 4.5450965 |
| C | 3.5474457 | -2.0856654 | 6.7082301 |
| H | 4.4924703 | -2.7569377 | 4.8802524 |
| H | 4.3160744 | -1.0075246 | 4.9970011 |
| H | 2.8366799 | -1.3008732 | 7.0277942 |
| H | 3.0440823 | -3.0480886 | 6.9182680 |
| C | 1.2362760 | -3.2201281 | 1.3786767 |
| C | 0.0815522 | -3.9160997 | 2.1089560 |
| H | 2.1232988 | -3.8740455 | 1.3651416 |
| H | 0.9593147 | -3.0252404 | 0.3321066 |
| C | -0.3055371 | -5.2470486 | 1.4551618 |
| H | 0.3597838 | -4.0768314 | 3.1652370 |

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| H | -0.7876914 | -3.2376372 | 2.1045963 |
| C | -1.5020809 | -5.9591784 | 2.1032696 |
| H | -0.5366623 | -5.0609434 | 0.3912851 |
| H | 0.5674368 | -5.9283500 | 1.4577113 |
| H | -1.7835441 | -6.8242567 | 1.4751148 |
| H | -2.3765173 | -5.2819467 | 2.0893318 |
| H | -1.6082071 | 3.0598413 | -2.1974478 |
| C | 2.9325796 | -5.7424815 | -7.4086178 |
| C | 2.1405502 | -6.1046002 | -8.6687092 |
| H | 2.7626917 | -6.5153410 | -6.6353986 |
| H | 4.0150248 | -5.7800113 | -7.6354836 |
| H | 1.0575296 | -6.0448804 | -8.4496811 |
| H | 2.3291571 | -5.3428704 | -9.4491693 |
| C | 2.4640315 | -7.4927060 | -9.2309342 |
| C | 1.6845346 | -7.8354833 | -10.5016979 |
| H | 2.2594735 | -8.2543547 | -8.4559670 |
| H | 3.5489707 | -7.5582904 | -9.4347744 |
| H | 1.9374910 | -8.8413813 | -10.8743330 |
| H | 0.5958065 | -7.8112077 | -10.3238277 |
| H | 1.9006386 | -7.1171155 | -11.3109962 |
| C | -5.6814297 | 3.3027564 | -3.3452583 |
| C | -6.5429748 | 2.1526175 | -3.8755420 |
| H | -5.8986486 | 4.2185429 | -3.9274875 |
| H | -5.9775195 | 3.5331655 | -2.3046345 |
| H | -6.2630132 | 1.9435589 | -4.9255749 |
| H | -6.3048067 | 1.2289060 | -3.3149345 |
| C | -8.0508079 | 2.4131344 | -3.7990402 |
| C | -8.8973582 | 1.2718634 | -4.3656886 |
| H | -8.2862317 | 3.3495634 | -4.3382643 |
| H | -8.3343579 | 2.5959635 | -2.7461640 |
| H | -9.9755021 | 1.4872447 | -4.2876518 |
| H | -8.6697152 | 1.0952272 | -5.4309042 |
| H | -8.7077023 | 0.3267408 | -3.8287873 |
| C | 3.4040368 | 3.9388584 | -8.1386904 |
| C | 3.5211384 | 2.9440754 | -9.2974373 |
| H | 4.4101595 | 4.1286696 | -7.7191213 |
| H | 3.0566748 | 4.9134184 | -8.5301755 |
| H | 3.8708625 | 1.9687468 | -8.9094052 |
| H | 2.5165747 | 2.7537217 | -9.7202457 |
| C | 4.4601690 | 3.4081579 | -10.4156767 |
| C | 4.5805058 | 2.4134923 | -11.5714666 |
| H | 5.4621446 | 3.6012876 | -9.9896601 |
| H | 4.1080298 | 4.3821834 | -10.8024259 |
| H | 5.2638183 | 2.7824101 | -12.3535317 |
| H | 4.9667822 | 1.4399223 | -11.2246934 |
| H | 3.6016910 | 2.2279409 | -12.0457061 |
| C | 4.8239388 | -1.9843391 | 7.5494926 |
| C | 4.5899212 | -2.1073333 | 9.0581520 |
| H | 5.3233109 | -1.0201216 | 7.3365194 |
| H | 5.5365802 | -2.7663165 | 7.2262083 |
| H | 3.8693739 | -1.3321921 | 9.3807875 |
| H | 4.1021441 | -3.0766765 | 9.2752640 |

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| C | 5.8680721 | -1.9859464 | 9.8949741 |
| C | 5.6307707 | -2.1102274 | 11.4010592 |
| H | 6.3525553 | -1.0160631 | 9.6768263 |
| H | 6.5887699 | -2.7588454 | 9.5699272 |
| H | 6.5702874 | -2.0139600 | 11.9690633 |
| H | 4.9409366 | -1.3294615 | 11.7644385 |
| H | 5.1858893 | -3.0866390 | 11.6584001 |
| C | -1.2667603 | -6.4499474 | 3.5367319 |
| C | -2.4574083 | -7.2056355 | 4.1347226 |
| H | -1.0238074 | -5.5939118 | 4.1917754 |
| H | -0.3735859 | -7.1036346 | 3.5543180 |
| H | -3.3525185 | -6.5556354 | 4.1074902 |
| H | -2.7012134 | -8.0741784 | 3.4935487 |
| C | -2.2281393 | -7.6868262 | 5.5712836 |
| C | -3.4210500 | -8.4360655 | 6.1674764 |
| H | -1.9828521 | -6.8174999 | 6.2093733 |
| H | -1.3339297 | -8.3368531 | 5.5975872 |
| H | -3.2191025 | -8.7651877 | 7.1998647 |
| H | -4.3225870 | -7.8003253 | 6.1915982 |
| H | -3.6689640 | -9.3334388 | 5.5749604 |
| C | 8.4883910 | 3.0291297 | -3.8780409 |
| C | 9.9150994 | 3.2008938 | -3.3477098 |
| H | 7.9116003 | 3.9524193 | -3.6810231 |
| H | 8.5174791 | 2.9245179 | -4.9790414 |
| H | 9.8832966 | 3.3145732 | -2.2475219 |
| H | 10.4864434 | 2.2718456 | -3.5335985 |
| C | 10.6717928 | 4.3865832 | -3.9549595 |
| C | 12.0921182 | 4.5467379 | -3.4100043 |
| H | 10.0996288 | 5.3151484 | -3.7733581 |
| H | 10.7089337 | 4.2692330 | -5.0537557 |
| H | 12.6093563 | 5.4046190 | -3.8692390 |
| H | 12.0870060 | 4.7069528 | -2.3183058 |
| H | 12.7004030 | 3.6474586 | -3.6064192 |
| C | 2.4388917 | 3.8864623 | -1.1859649 |
| C | 1.2328738 | 0.5334339 | 2.2186191 |
| C | 2.0234992 | 0.3033576 | -1.6060401 |
| C | 2.8354758 | 3.1903072 | 0.1362605 |
| H | 2.7399430 | 3.2694890 | -2.0484486 |
| H | 3.0324812 | 4.8157416 | -1.2680476 |
| H | 1.9333199 | 1.1153128 | -2.3430054 |
| H | 1.0140283 | 0.0596522 | -1.2464008 |
| H | 0.4630291 | 0.7324372 | 2.9842755 |
| H | 2.2069726 | 0.5814278 | 2.7226710 |

UO2$(NO_3)_2$-(HONTA)

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| N | 13.2719512 | 6.3944778 | 7.8450115 |
| C | 14.3586277 | 6.3805285 | 6.8932383 |
| H | 14.4852402 | 7.3890228 | 6.4661008 |
| H | 15.3269943 | 6.1461154 | 7.3761387 |
| C | 13.4118630 | 5.5072301 | 8.9843709 |

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| H | 13.5702704 | 6.0661960 | 9.9187698 |
| H | 14.3049430 | 4.8741776 | 8.8300765 |
| C | 12.6921039 | 7.7205465 | 8.0390052 |
| H | 12.4833773 | 8.1287633 | 7.0429165 |
| H | 13.4099893 | 8.4211759 | 8.5311065 |
| C | 14.1601490 | 5.4194698 | 5.7018943 |
| C | 12.2273304 | 4.5424993 | 9.1544640 |
| C | 11.4150810 | 7.7617012 | 8.8909476 |
| O | 11.2118290 | 6.8993535 | 9.7438336 |
| O | 13.0942018 | 4.7929846 | 5.5765608 |
| O | 11.5235168 | 4.2641408 | 8.1618494 |
| N | 12.0024403 | 3.9355722 | 10.3239528 |
| N | 10.5794528 | 8.8233366 | 8.7319406 |
| N | 15.1456339 | 5.2813801 | 4.7999501 |
| C | 10.8365852 | 3.0367313 | 10.4348491 |
| C | 11.1320857 | 1.5999917 | 9.9913455 |
| H | 10.0188508 | 3.4635458 | 9.8368347 |
| H | 10.5157840 | 3.0537807 | 11.4879608 |
| C | 9.9108306 | 0.6854525 | 10.1313339 |
| H | 11.4623599 | 1.6129112 | 8.9393650 |
| H | 11.9727293 | 1.1927488 | 10.5839909 |
| C | 10.1673508 | -0.7518203 | 9.6670415 |
| H | 9.5742019 | 0.6764316 | 11.1854538 |
| H | 9.0733367 | 1.1119470 | 9.5501676 |
| H | 10.4974020 | -0.7367028 | 8.6121524 |
| H | 11.0121295 | -1.1776177 | 10.2414597 |
| C | 12.8175549 | 4.1321910 | 11.5257007 |
| C | 12.2549675 | 5.1658774 | 12.5086754 |
| H | 13.8426356 | 4.4038327 | 11.2347029 |
| H | 12.9033504 | 3.1499011 | 12.0199121 |
| C | 13.1474918 | 5.3372431 | 13.7412163 |
| H | 12.1185737 | 6.1253641 | 11.9837837 |
| H | 11.2445140 | 4.8518493 | 12.8234376 |
| C | 12.5893929 | 6.3215937 | 14.7739345 |
| H | 13.3026251 | 4.3540227 | 14.2246280 |
| H | 14.1528985 | 5.6744959 | 13.4240307 |
| H | 12.4261569 | 7.3031010 | 14.2911884 |
| H | 11.5893677 | 5.9784963 | 15.0977959 |
| C | 14.9246895 | 4.3819153 | 3.6426519 |
| C | 15.0740095 | 2.8867599 | 3.9491802 |
| H | 15.6466456 | 4.6859839 | 2.8694743 |
| H | 13.9167264 | 4.5706384 | 3.2441891 |
| C | 14.8527804 | 2.0305098 | 2.6962386 |
| H | 16.0736525 | 2.6826257 | 4.3747991 |
| C | 14.8672135 | 0.5242542 | 2.9743601 |
| H | 13.8876424 | 2.3084377 | 2.2389577 |
| H | 15.6274495 | 2.2734102 | 1.9439372 |
| H | 15.8394349 | 0.2343233 | 3.4181323 |
| H | 14.1037133 | 0.2935764 | 3.7398709 |
| C | 16.4292688 | 5.9873954 | 4.8902427 |
| C | 17.5586340 | 5.1831543 | 5.5466634 |
| H | 16.2931491 | 6.9398753 | 5.4225100 |

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| H | 16.7196389 | 6.2607495 | 3.8634589 |
| C | 18.8792217 | 5.9577564 | 5.5941411 |
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| H | 17.7000104 | 4.2371152 | 4.9973385 |
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| H | 12.0603508 | 1.6431374 | -3.0919738 |
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| H | 10.9670264 | 2.3730169 | -5.8781056 |
| C | 8.1141128 | -3.0273803 | 1.5466425 |
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| C | 8.3912550 | -2.7150587 | 4.0125319 |
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| C | 9.1161819 | -4.4506534 | 5.7082913 |
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| H | 8.0467174 | -4.6559964 | 5.9099743 |
| H | 9.8766517 | -5.8951317 | 7.1169447 |
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| H | 7.1968705 | 9.4959856 | 4.6893641 |
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| H | 10.1333309 | -8.3800204 | 6.8175400 |
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| H | 10.2515500 | -11.6574397 | 4.8951727 |
| H | 11.6707594 | -10.6588519 | 5.2875549 |
| H | 10.4272834 | -10.9584783 | 6.5215615 |
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| H | -0.2441214 | -1.1297890 | 2.3532162 |
| H | -0.9378284 | 0.1731547 | 3.3171249 |
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| H | -1.7848704 | -0.5452871 | 0.4470832 |
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| H | -2.6064242 | -2.2339207 | 2.1566821 |
| H | -3.3062948 | -0.9117315 | 3.1162100 |
| N | 7.3204276 | 1.4065405 | 6.4042929 |
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| N | 10.1493850 | 4.8609843 | 2.8577847 |

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| O | 8.3213397 | 1.0180693 | 5.6707423 |
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| O | 12.8397807 | 2.7585321 | 1.8910407 |
| O | 11.8743534 | 1.4602767 | 0.4560852 |
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$UO2(NO_3)_2$-(HONTA-C2)$_2$

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| C | 13.6088250 | 2.6351391 | 5.3321303 |
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| H | 13.6458655 | 1.8251478 | 6.0715266 |
| C | 13.7030097 | 3.2053439 | 8.2361898 |
| H | 14.0972174 | 3.7827709 | 9.0835361 |
| H | 14.5182543 | 2.5482763 | 7.9005272 |
| C | 12.5474575 | 4.7693385 | 4.9155912 |
| H | 12.0611406 | 4.3066966 | 4.0519439 |
| H | 13.5087998 | 5.2018756 | 4.5495825 |
| C | 13.9151959 | 0.8563533 | 3.5237579 |
| C | 12.5469430 | 2.2859164 | 8.6304200 |
| C | 10.2194266 | 5.6568044 | 5.6128695 |
| O | 9.5648962 | 4.9599137 | 4.8084861 |
| O | 13.5199455 | -0.3012960 | 3.6226749 |
| O | 12.2562333 | 1.3363770 | 7.9162321 |
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| C | 10.6305865 | 1.7376595 | 10.0080302 |
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| H | 11.9801025 | 2.9523237 | 11.8045951 |
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| H | 10.1972846 | 6.9471162 | 12.0578500 |
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| C | 16.6649452 | -0.7801757 | 3.5993603 |
| H | 16.6285533 | 0.3204752 | 1.7255321 |
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| H | 19.5026219 | 3.9239966 | 3.4789272 |
| C | 10.2794762 | 7.0807061 | 7.6562701 |
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| H | 5.6424086 | 6.5765867 | 7.7609142 |
| H | 3.6885998 | 6.9450823 | 6.2037614 |
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| H | 22.6221094 | 9.2763570 | 4.1275631 |
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| H | 23.1008187 | 7.5664338 | 4.2330734 |
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| H | 12.5553175 | 11.4845686 | 9.3604492 |
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| C | 12.0092085 | 15.6684694 | 9.6857645 |

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| H | 9.6198241 | 11.4281295 | 14.5752503 |
| N | 10.1100522 | 1.0524053 | -0.1084308 |
| C | 11.1723948 | 3.1914234 | -1.0877451 |
| H | 12.2046856 | 3.5519836 | -1.1949439 |
| H | 10.8549755 | 2.8840879 | -2.0989291 |
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| H | 8.7933793 | 2.3242776 | -1.0960703 |
| C | 10.4850680 | -0.3230123 | 0.1653401 |
| H | 11.5054221 | -0.5071740 | -0.2279392 |
| H | 9.8280205 | -0.9924535 | -0.4179873 |
| C | 10.3101191 | 4.3676496 | -0.6539939 |
| C | 6.9043673 | 1.6577435 | 0.7051392 |
| C | 9.3446863 | -1.7413922 | 1.9820128 |
| O | 8.2277639 | -1.3459527 | 2.3168652 |
| O | 9.4447950 | 4.2236749 | 0.2303483 |
| O | 7.5176511 | 2.5714473 | 1.2949451 |
| N | 5.5809707 | 1.4832366 | 0.9059448 |
| N | 9.5911634 | -3.0907770 | 1.8512661 |
| N | 10.4532591 | 5.5537005 | -1.2938912 |
| C | 4.8514296 | 2.4040338 | 1.7935743 |
| C | 4.2917918 | 3.6222054 | 1.0505081 |

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| H | 4.0318080 | 1.8324433 | 2.2560582 |
| C | 3.3967846 | 4.4902886 | 1.9400883 |
| H | 5.1367261 | 4.2231983 | 0.6721439 |
| H | 3.7192017 | 3.2865456 | 0.1645177 |
| C | 2.8263780 | 5.7150676 | 1.2194046 |
| H | 2.5612470 | 3.8748554 | 2.3249252 |
| H | 3.9706813 | 4.8092503 | 2.8266922 |
| H | 3.6599452 | 6.3529551 | 0.8702337 |
| H | 2.2951231 | 5.3887997 | 0.3044382 |
| C | 4.7848166 | 0.3923155 | 0.3357983 |
| C | 4.7023484 | -0.8563420 | 1.2237075 |
| H | 5.1712163 | 0.1163414 | -0.6540526 |
| H | 3.7723311 | 0.7912467 | 0.1588249 |
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| H | 2.4030319 | 6.8832458 | 2.9928467 |
| H | 1.0446484 | 5.9102050 | 2.4316301 |
| H | 2.1245176 | 8.4250988 | 1.0219351 |
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| C | 0.3139702 | 8.5908403 | 2.1967595 |
| C | -0.2621237 | 9.8009714 | 1.4593478 |
| H | 0.8197875 | 8.9280267 | 3.1201566 |
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| H | -0.9698096 | 10.3632395 | 2.0901324 |
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| H | 12.9621153 | 2.7687876 | 3.2316768 |
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| C | 13.8347270 | 7.1872824 | 7.1885339 |
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| H | 14.0161250 | 2.5472058 | 1.6503597 |
| H | 12.6594725 | 3.0037582 | 2.6795178 |
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| H | 17.9573993 | 3.6791275 | 0.9306620 |
| H | 18.4176435 | 4.7732417 | 2.2340496 |
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| H | 24.2142118 | 0.9773778 | 0.9650173 |
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| O | 10.8307561 | 3.6046618 | 7.8378020 |
| O | 9.8868940 | 2.7014967 | 9.5671831 |
| O | 13.2115838 | 7.3529914 | 3.2000247 |
| O | 11.0861951 | 7.1252637 | 2.8396519 |
| O | 11.9500317 | 6.5204772 | 4.7518383 |
| O | 9.0261116 | 4.4858714 | 8.6965469 |
| C | 14.0321250 | 5.4155226 | 8.8318704 |

| | | | |
|---|---|---|---|
| H | 14.6830292 | 6.1728582 | 9.3227725 |
| H | 13.0285891 | 5.5286997 | 9.2718843 |
| C | 12.9035720 | 7.9868347 | 8.1073771 |
| C | 15.0179174 | 5.3380993 | 5.1024031 |
| H | 16.0515255 | 5.2571826 | 4.7462267 |
| H | 14.6478791 | 6.3192343 | 4.7629494 |
| Pu | 11.0827550 | 4.8147862 | 5.9405247 |
| H | 15.1560238 | 4.1331944 | 6.8637482 |
| H | 14.8430216 | 7.6404427 | 7.3247154 |
| H | 12.9740101 | 9.0378954 | 7.7864089 |
| H | 13.2708571 | 7.9786291 | 9.1470088 |
| H | 13.5337801 | 7.3717327 | 6.1500879 |

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