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Thèse

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par

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Filière : chimie des matériaux

Annexes

Synthèse et étude cristallochimique de carboxylates d'actinides tétravalents (Th, U, Np) : polymères de coordination et entités moléculaires à haute nucléarité

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Annexes

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I. Annexes expérimentales

I.1 Optimisation de la synthèse du composé Th-bdc

En vue d'obtenir des cristaux du composé Th-bdc de taille suffisante pour être analysable par diffraction des rayons-X sur monocristal, différentes synthèses ont été entreprises. Nous avons principalement modifié la température mais aussi le temps de chauffage. Des essais ont aussi été réalisés avec des concentrations en métal et/ou en ligand plus élevées. Le Tableau 1 présente toutes les conditions opératoires des différents tests que nous avons effectués.

Tableau 1: Liste des essais de synthèse en vue d'augmenter la taille des cristaux du composé Th-1,2-bdc).

Source métallique	**Ligand**	**Solvant**	**Température**	**Durée de chauffage**
$Th(NO_3)_4{\cdot}5H_2O$ 200 mg *0,35 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	150°C	24h
$Th(NO_3)_4{\cdot}5H_2O$ 400 mg *0,70 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	150°C	24h
$Th(NO_3)_4{\cdot}5H_2O$ 200 mg *0,35 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	100°C	24h
$Th(NO_3)_4{\cdot}5H_2O$ 400 mg *0,70 mmol*	1,2-H_2btc 220 mg *1,22 mmol*	H_2O 4mL *222 mmol*	100°C	24h
$Th(NO_3)_4{\cdot}5H_2O$ 200 mg *0,35 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	130°C	3j
$Th(NO_3)_4{\cdot}5H_2O$ 200 mg *0,35 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	130°C	5j
$Th(NO_3)_4{\cdot}5H_2O$ 200 mg *0,35 mmol*	1,2-H_2btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	180°C	24h
$Th(NO_3)_4{\cdot}5H_2O$ 400 mg *0,70 mmol*	1,2-H_2btc 220 mg *1,22 mmol*	H_2O 4mL *222 mmol*	180°C	24h

$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2-*H*$_2$btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	180°C	3j
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2-*H*$_2$btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	210°C	24h
$Th(NO_3)_4 \cdot 5H_2O$ 400 mg *0,70 mmol*	1,2-*H*$_2$btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	210°C	24h

Toutes les synthèses présentées ont conduit à la formation d'une poudre blanche. La diffraction des rayons-X sur poudre révèle que le composé Th-bdc inconnu cristallise dans tous les cas. Aucune synthèse n'a permis de générer des cristaux suffisamment gros en vue de leurs analyses par diffraction des rayons X sur monocristal. Comme décrit lors du chapitre II, la synthèse ayant suivi un traitement à 180°C pendant 3j présente un second composé : $Th(OH)(H_2O)$(1,2,3-btc).

I.2 Essais de synthèse du composé $Th(OH)(H_2O)$(1,2,3-btc)

Lors de nos essais avec le thorium et l'acide phtalique nous avons isolé un composé cristallisé présentant en son sein le ligand 1,2,3-benzène tricarboxylique (1,2,3-H_3btc). Différents essais ont été réalisés, dans le but d'améliorer les conditions de synthèse de ce composé, en utilisant le ligand phtalate (1,2-bdc) ou directement avec le ligand 1,2,3-btc. La liste des synthèses et les résultats obtenus sont regroupés dans le Tableau 2. La synthèse originale est également donnée pour comparaison.

Tableau 2: Liste des essais de synthèse en vue d'obtenir le composé $Th(OH)(H_2O)$(1,2,3-btc).

Source métallique	**Ligand**	**Solvant**		**Temps et température**	**Résultats obtenus**
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2-*H*$_2$btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	-	72h 180°C	Composés Th-bdc et $Th(OH)(H_2O)$(1,2,3-btc)
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2-*H*$_2$btc 110 mg *0,66 mmol*	H_2O 4mL *222 mmol*	-	24h 220°C	Composé Th-bdc
$Th(NO_3)_4 \cdot 5H_2O$ 400 mg *0,70 mmol*	1,2-*H*$_2$btc 230 mg *1,38 mmol*	H_2O 4mL *222 mmol*	-	24h 180°C	Composé Th-bdc

$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2,3-*H*$_3$btc 70 mg *0,33 mmol*	H_2O 4mL *222 mmol*	-	24h 180°C	Poudre blanche amorphe
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2,3-*H*$_3$btc 70 mg *0,33 mmol*	H_2O 4mL *222 mmol*	-	24h 150°C	Poudre blanche amorphe
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2,3-*H*$_3$btc 70 mg *0,33 mmol*	H_2O 4mL *222 mmol*	NaOH (4M) 0,25 mL *1 mmol*	24h 150°C	Poudre blanche amorphe
$Th(NO_3)_4 \cdot 5H_2O$ 200 mg *0,35 mmol*	1,2,3-*H*$_3$btc 70 mg *0,33 mmol*	H_2O 4mL *222 mmol*	NaOH (4M) 1 mL *4 mmol*	24h 150°C	Poudre blanche amorphe

I.3 Synthèses des ligands fonctionnalisés

I.3.1 NH_2-bpdc

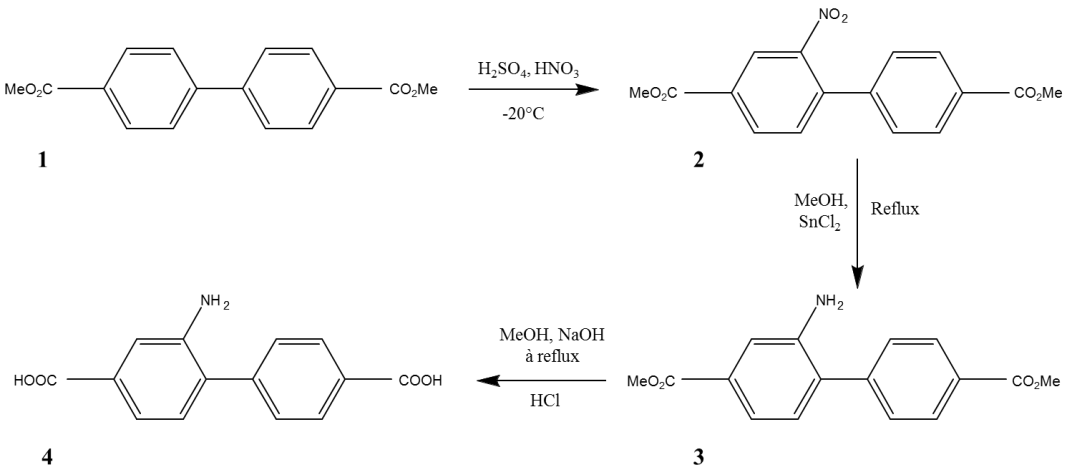


Figure 1:Schéma réactionnel de la synthèse du ligand NH_2-bpdc

Nitration

A une solution de 2,53 g de biphényle-4,4'-dicarboxylate de diméthyle dans 27 mL d'H_2SO_4 concentrée placée à -20°C est ajoutée goutte à goutte un mélange nitreux composé de 1,3 mL d'HNO_3 (65 %) et 4 mL d'H_2SO_4. La solution est ensuite agitée pendant 1h entre -20 et -10°C avant de remonter la température à 0°C pendant 30 min. Le solide rosé ainsi formé est filtré puis dissout dans du dichlorométhane. La phase organique est lavée avec de l'eau puis avec une solution aqueuse de $NaHCO_3$ saturée, avant d'être séchée sur du $MgSO_4$. L'évaporation sous pression réduite du solvant permet ainsi d'isoler le dérivé mononitro.

Réduction

Une solution composée du produit précédemment obtenu, 4 équivalents en masse de $SnCl_2$ dans 25 mL de méthanol est portée à reflux pendant une nuit. Le volume de la solution est ensuite réduit de moitié à l'aide d'un évaporateur rotatif. Après recristallisation, le dérivé monoamino est isolé par filtration du mélange.

Saponification

Le produit ainsi récupéré est dissout dans un mélange contenant 20 mL de méthanol et 20 mL d'une solution aqueuse de NaOH (2 M) et porté à reflux pendant une nuit. Le méthanol est ensuite évaporé sous pression réduite. Le mélange obtenu est acidifié jusqu'à pH = 1 avec une solution d'acide chlorhydrique (6M). Le solide précipité obtenu est filtré et lavé avec de l'eau. Le produit souhaité est ainsi obtenu sous forme de sel d'ammonium.

La mesure RMN liquide du proton de ce ligand a été réalisée sur un spectromètre Bruker AvanceII (^{1}H = 300 MHz) à 300 K équipé d'une sonde 5 mm QNP. Le ligand a été dissous dans du DMSO deutéré

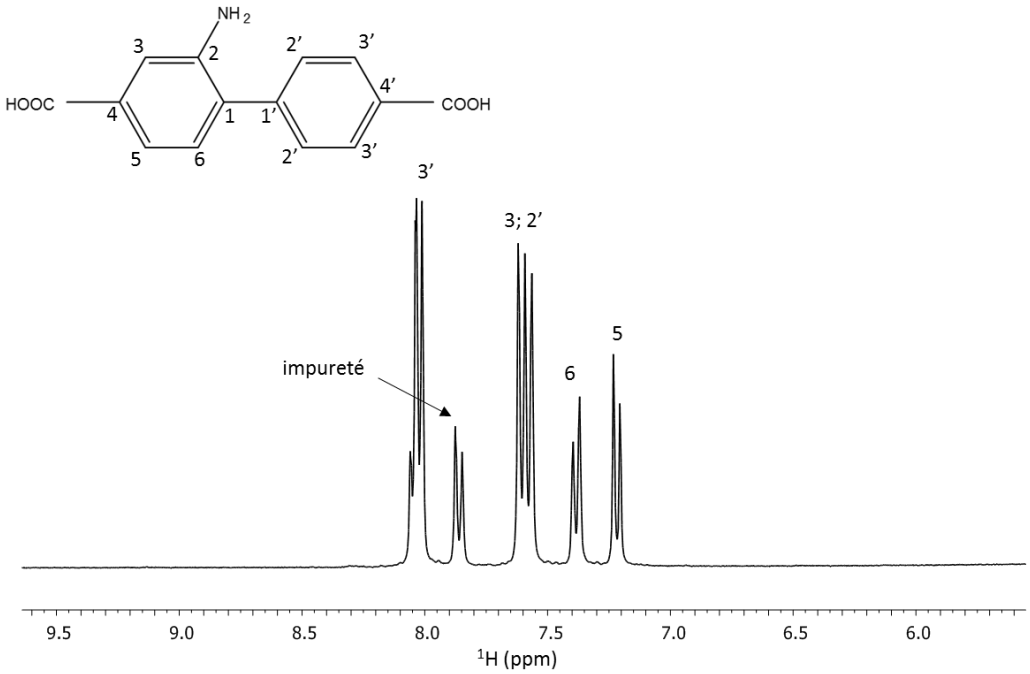


Figure 2: Spectre ^{1}H du composé NH_2-bpdc dans le DMSO deutéré.

I.3.2 NH_2-tpdc

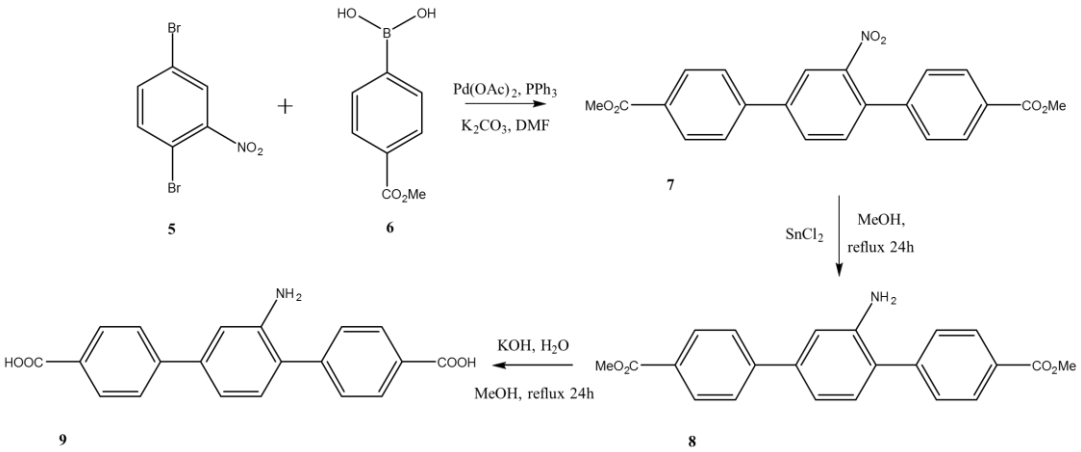


Figure 3: Schéma réactionnel de la synthèse du ligand NH_2-tpdc

Couplage

Un mélange contenant 200 mg (0,7 mmol) de 2,5-dibromo-nitrobenzène, 350 mg (1,9 mmol) d'acide 4-méthoxycarboxybenzène boronique, 4 mg $Pd(OAc)_2$ et 20 mg de triphénylphosphine et 5,5 mL de DMF est placé dans un tube schlenk de 50 mL. La solution est dégazée en réalisant des cycles de « freeze pump » avant d'être placée pour une nuit à 95°C et sous agitation. La solution est ensuite placée à 0°C sous agitation et le solide marron beige obtenu est isolé par filtration puis lavé avec de l'eau. Le solide est ensuite dissout dans du dichlorométhane et la solution ainsi obtenue est lavée avec une solution aqueuse de HCl (3M) puis avec une solution saturée de NaCl. La solution organique est filtrée sur célite, avant d'être évaporée sous pression réduite. Une recristallisation dans l'acétonitrile du solide obtenu conduit à la formation du ligand **7**.

Réduction

Le ligand **7** isolé précédemment est mis en suspension dans 20 mL de mélange méthanol/dichlorométhane, en présence de 4 équivalents $SnCl_2$ et de quelques gouttes d'acide chlorhydrique concentré. Le mélange est porté à reflux, sous agitation, pendant 24h. Une solution aqueuse de soude (6M) est ensuite ajoutée afin de basifier le système jusqu'à un pH de 9-10. Le solide jaune (**8**) ainsi précipité est isolé par filtration, lavé avec du méthanol puis séché.

Saponification

Le ligand **8** est dissout dans 20 mL de méthanol en présence de 5 mL de KOH (2M). La solution est placée sous agitation et à reflux pour une nuit. Après avoir évaporé le méthanol sous pression réduite, la solution est acidifiée jusqu'à pH = 1 par ajout d'une solution d'acide chlorhydrique (6M). Le solide jaune correspondant au produit **9** est récupéré par filtration, lavé avec environ 30 mL d'eau et séché.

La mesure RMN liquide du proton de ce ligand a été réalisée sur un spectromètre Bruker AvanceII (^{1}H = 300 MHz) à 300 K équipé d'une sonde 5 mm QNP. Le ligand a été dissout dans du DMSO deutéré.

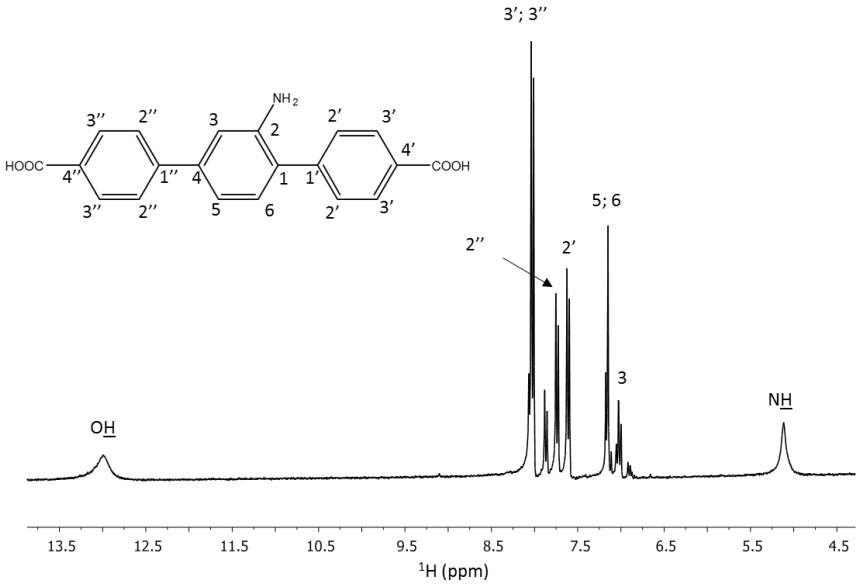


Figure 4: Spectre ^{1}H du composé NH_2-tpdc dans le DMSO deutéré.

I.4 RMN composé U_{38}-iPrOH

Une étude RMN des solutions surnageantes a été effectuée dans l'optique d'observer la présence d'eau ou d'ester en solution, confirmant ainsi notre hypothèse de réaction d'estérification. Les solutions surnageantes issues des différentes synthèses ont été analysées à 285 K par RMN liquide du proton sur un spectromètre Bruker AvanceII 400 (^{1}H = 400 MHz) équipé d'une sonde TBI 5 mm ou d'une sonde BBO 10 mm. Les échantillons analysés ont été introduits dans des inserts coaxiaux placés dans des tubes standards contenant de l'acétonitrile deutéré (ACN-d3, enrichissement isotopique à 99,8%,

Eurisotop) permettant les réglages de la machine (lock et shims). Le choix d'une référence externe est d'observer toutes les espèces présentes en solution sans affecter notre système.

Avant d'analyser nos échantillons, nous avons mesuré des solutions de diverses compositions, chauffées à 100 °C pendant 24 h. Des solutions avec et sans uranium, et avec différentes concentrations en acide ont été analysées afin de séparer plus facilement tous les signaux ^{1}H observés. Des mesures de proton 1D ou 2D (COSY) ainsi que des corrélations 2D ^{1}H-^{13}C (HSQC et HMBC) nous ont permis d'attribuer tous les pics observés sur les spectres obtenus. Il est à noter que la modification de certains paramètres comme par exemple la concentration, l'acidité, la température induisent des décalages de pics. Selon le pic considéré et les conditions de mesure et de synthèse, ce décalage peut être plus ou moins prononcé. Par exemple, le signal du proton de la fonction alcool est déplacé vers la gauche lorsque l'acidité du milieu augmente. Etant donné que toutes nos mesures n'ont pas été réalisées sur le même échantillon, ces décalages sont observés sans que cela affecte l'analyse et l'interprétation des résultats. Cependant, dans notre cas, les positions relatives de tous les signaux restent inchangées.

Pour commencer, nous avons analysé une solution chauffée 24 h à 100 °C contenant initialement 150 mg d'acide benzoïque et 1 mL de solvant isopropanol. Nous avons fait le choix d'utiliser une quantité d'acide benzoïque plus importante que celle reportée pour la synthèse du composé (30 mg**Error! Reference source not found.**) afin de mieux observer l es zones d'intérêts. La Figure 5 présente le spectre ^{1}H obtenu.

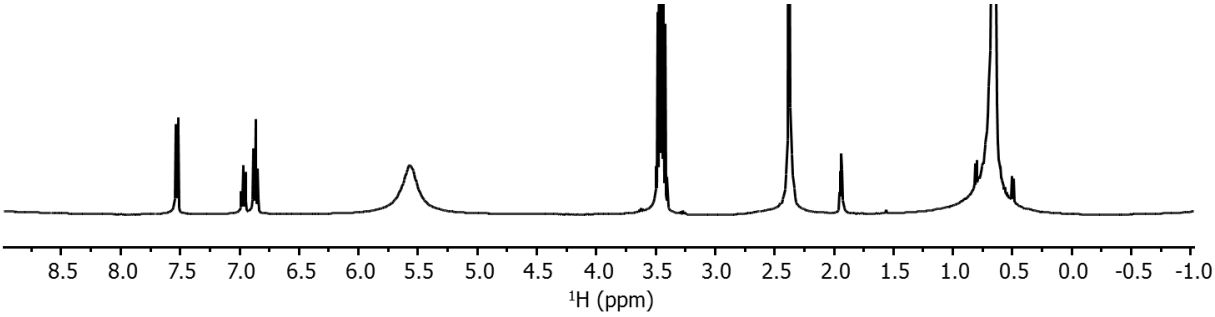
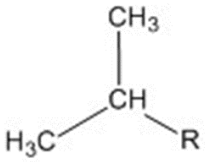


Figure 5: Spectre ^{1}H d'une solution chauffée 24h à 100°C contenant initialement 150 mg d'acide benzoïque et 1 mL de solvant isopropanol. Sonde BBO 10 mm.

Les pics possédant les surfaces les plus importantes correspondent à notre solvant (ici l'isopropanol). Les protons des deux groupements CH_3 sont équivalents et apparaissent dans la région des faibles déplacements chimiques (entre 0,5 et 1 ppm environ) et sont observables sous la forme de doublets tandis que ceux des groupements CH apparaissent comme des septuplets vers 3,5 ppm. Le proton de la fonction alcool étant labile, sa position

peut fortement varier, mais il se situe généralement entre 5 et 6 ppm. La multiplicité (m) d'un signal proton peut être calculée selon l'équation (Equ. 1) suivante (où n correspond au nombre de partenaire observés et I le spin des partenaires) :

$$m = 2 * n * I + 1 \qquad \text{(Equ. 1)}$$



Au travers des constantes de couplages de type $^{3}J_{^{1}H\text{-}^{1}H}$, chaque proton des CH_3 (identiques du point de vue de la RMN) voit le proton du CH (n = 1) tandis que celui du CH voit six protons équivalents provenant des deux groupements méthyles. Le spin du proton étant égal à ½, la multiplicité est donc bien de 2 pour les protons des CH_3 et de 7 pour ceux du CH. Le proton du groupement OH devrait en théorie apparaitre sous la forme d'un doublet mais il est en échange, ce qui ne permet pas d'observer ces constantes de couplages. C'est également pour cette raison qu'il apparait comme un unique pic large à 5,5-5,7 ppm.

Dans la région entre 6,5 et 8 ppm, nous observons les protons appartenant aux cycles benzéniques. Trois massifs distincts correspondent aux protons situés en position *ortho*, *méta* et *para*. Le massif du milieu, le moins intense (sa surface est environ deux fois plus faible que celles des deux autres massifs) correspond à la position para. Il n'existe qu'un seul proton en position *para* alors qu'il en existe deux pour chacune des positions *ortho* et *meta*. Une expérience de type COSY a ensuite été enregistrée dans le but d'attribuer ces massifs aux deux positions restantes. Cette méthode consiste à déterminer pour un atome donné les corrélations existant entre divers signaux appartenant à un même motif chimique (appelé système de spins). Grâce à cette méthode 2D $^{1}H\text{-}^{1}H$, nous pouvons observer les protons voisins *via* des couplages scalaires $^{3}J_{^{1}H\text{-}^{1}H}$ et ainsi déterminer quels protons sont proches les uns des autres. Les pics observés sur la Figure 5 et sur la Figure 6 ne sont pas situés aux mêmes déplacements chimiques car les deux analyses ont été réalisées sur deux solutions de compositions différentes. Mais ici seules les positions relatives de ces trois massifs nous importent.

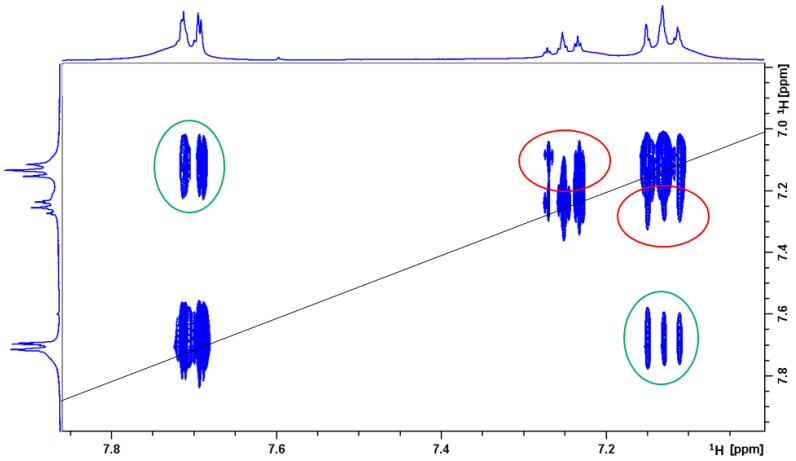


Figure 6 : Attribution des protons du cycle aromatique grâce à la 2D ^{1}H-COSY. Sonde BBO 10 mm.

Les taches de corrélations les plus intenses (sur la diagonale) correspondent à l'autocorrélation et ne sont pas utiles ici. On observe aussi des taches au niveau des intersections des déplacements chimiques à 7,13 et 7,70 ppm (et inversement) (cercles verts) et à 7,13 et 7,26 ppm (cercles rouges). Etant donné que le massif du centre (ici à 7,26 ppm) avait été attribué au proton en position *para* du cycle aromatique, nous pouvons affirmer que le massif centré à 7,13 ppm correspond aux protons en position *meta*. La corrélation à 7,13/7,70 ppm nous confirme que ces protons appartiennent au même système de spin et par conséquent que le massif à 7,70 ppm correspond aux protons en *ortho* du cycle benzénique.

Il est important de souligner qu'autour des pics ^{1}H des groupements CH_3 et CH appartenant à l'alcool libre, il est possible de distinguer d'autres massifs de part et d'autre du massif principal. Ces pics mineurs sont les signaux des protons liés à un ^{13}C (et non un ^{12}C). Ils sont largement minoritaires car cet isotope ^{13}C n'existe naturellement qu'à hauteur de 1,1%. Ces pics appelés satellites possèdent la même forme que le pic principal et sont séparés d'environ 130 Hz (pour les CH_3) ou 140-150 Hz (pour les CH) ce qui correspond à la constante de couplage $^{1}J_{^{1}H-^{13}C}$.

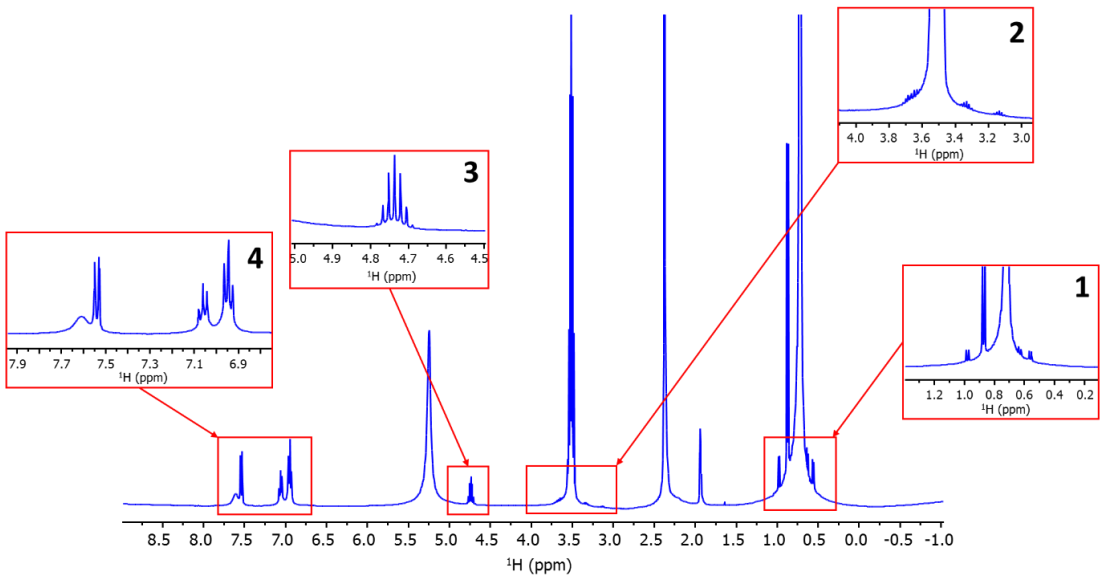


Figure 7: Spectres ^{1}H d'une solution chauffée 24h à 100°C contenant initialement 10 mg d'UCl_4, 150 mg d'acide benzoïque et 1 mL de solvant isopropanol. Les zones 1 à 4 ont été zoomées et montrent les régions d'intérêts. Sonde TBI 5mm.

La Figure 7 montre le spectre proton d'une solution contenant 10 mg d'UCl_4 associés aux mêmes quantités de réactifs (acide benzoïque et isopropanol) que celui montré dans la Figure 5. La comparaison de ces deux spectres permet de mettre en évidence que l'ajout d'uranium au mélange réactionnel génère des signaux protons supplémentaires. Un doublet fin et intense apparait à 0,87 ppm juste à gauche des signaux protons des groupements CH_3 de l'alcool libre (zone 1), tandis qu'un massif composé de sept pics est observable vers 4,74 ppm (zone 3). Ce dernier possède la même allure que le massif des protons des CH de l'alcool libre mais le décalage est bien plus prononcé que pour les groupements CH_3. Une expérience 2D de type COSY montre que ces deux pics sont corrélés signifiant qu'ils appartiennent au même système de spin. Une analyse HSQC (*heteronuclear single quantum correlation*) permet de déterminer les déplacements chimiques de deux atomes différents (ici ^{1}H et le ^{13}C) directement liés entre eux. Ceci révèle que le proton des CH de cette espèce corrèle un ^{13}C situé à 68,9 ppm tandis que celui appartenant à l'alcool libre corrèle un ^{13}C à 63,5 ppm. Le fait que le déplacement chimique de cet atome de carbone des groupements CH augmente par rapport à celui appartenant à l'alcool signifie qu'il est substitué. Toutes ces informations montrent que le motif isopropyle est toujours présent au sein de cette espèce et qu'il s'agit surement de la forme ester attendue : le benzoate d'isopropyle. Afin de confirmer cette hypothèse, nous avons réalisé une mesure de type HMBC (*heteronuclear multiple bond correlation*) qui consiste à corréler deux noyaux différents (dans ce cas le ^{1}H et le ^{13}C) *via* des interactions de type ^{3}J d'environ 10 Hz. Par cette méthode, nous avons montré une corrélation entre le proton

situé à 4,74 ppm (issu des CH) et un carbone situé à 166 ppm. Ce dernier se situe dans la région typique des atomes de carbone carboxyle. Ce même carbone est aussi corrélé à un proton en position *ortho* d'un cycle benzénique (situé à 7,54 ppm) et plus faiblement à celui en position *meta* (situé à 6,95 ppm). Ces deux informations nous permettent de dire que ces protons appartenant au cycle benzénique et au groupement isopropyle substitué font parties de la même molécule, le lien étant la fonction ester attendue.

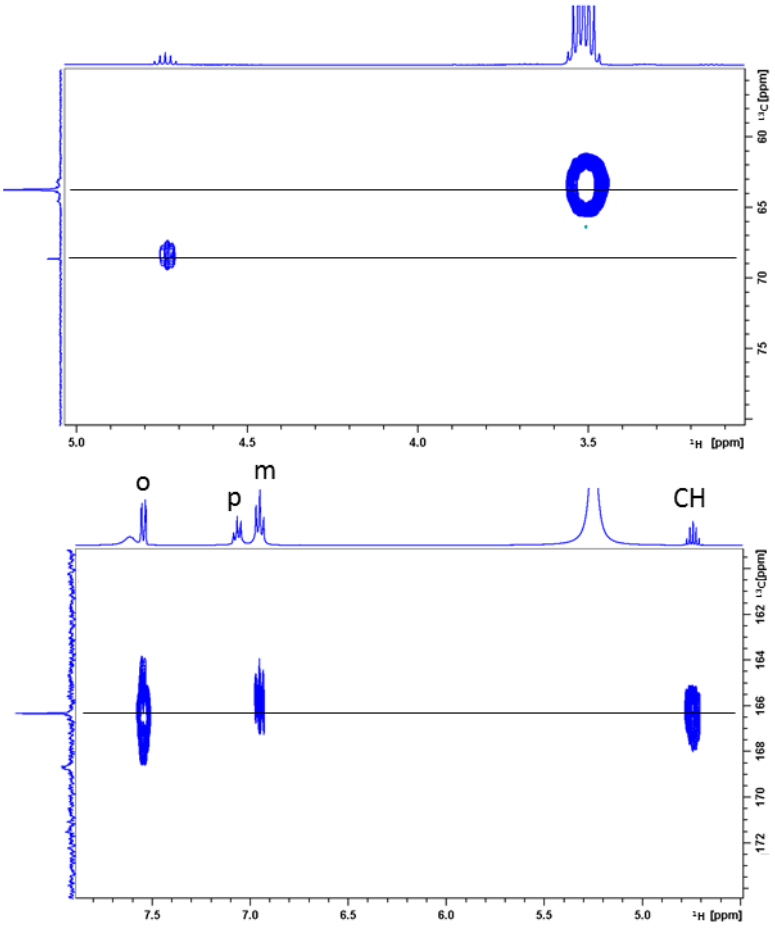


Figure 8: Spectres 2D ^{1}H-^{13}C d'une solution chauffée 24h à 100°C contenant initialement 10 mg d'UCl_4, 150 mg d'acide benzoïque et 1 mL de solvant isopropanol : (haut) HSQC ; (bas) HMBC. Sonde BBO 10 mm.

Ceci signifie également que les groupements CH des cycles aromatiques visibles entre 6 et 8 ppm appartiennent à la forme ester. Pour le moment, nous n'avons pas été capable de distinguer dans cette région la forme acide libre de la forme ester, les deux formes semblent être confondues. Les protons ne sont pas assez affectés pour générer des variations de déplacements chimiques suffisantes permettant une bonne séparation. Cependant on peut noter la présence d'un signal très large (vers 7,6 ppm), légèrement décalée vers la gauche par rapport au pic du proton en position *ortho* (7,54 ppm) (zone 4). Dans des conditions bien particulières (large excès d'acide benzoïque), il est possible de deviner des pics similaires très proches à gauche (sous la forme d'un épaulement) voire

confondus avec les signaux des deux autres protons *meta* et *para* des cycles benzéniques. On note que ce décalage des pics ainsi que cet élargissement est d'autant plus prononcé lorsque le proton se trouve proche de la fonction carboxylate. Ceci semble être l'œuvre d'un métal paramagnétique proche de cette fonction. Dans notre cas seul l'uranium tétravalent est paramagnétique, ce qui tend à dire que ces pics appartiennent aux protons issus d'un benzoate d'uranium. Le fait que ce phénomène de décalage et d'élargissement soit plus marqué dans le cas où les solutions ont suivi un traitement thermique court, et donc où la concentration en uranium est importante, confirme notre hypothèse. Il n'est cependant pas possible par cette méthode de dire combien de groupements benzoate sont reliés à un atome d'uranium.

Dans les zones 1 et 2 de la Figure 7, il est possible de remarquer la présence d'autres signaux très faibles. Ceux situés dans la région des groupements CH_3 à 0,56 et 0,87 ppm (confondu avec le signal de l'ester) et dans la région des groupements CH à 3,33 et 3,68 (chevauchement avec un autre signal) ont été précédemment attribués aux signaux satellites (proton lié à un ^{13}C) appartenant à l'alcool libre. Cependant, des doublets supplémentaires sont observés à 0,63 et 0,98 ppm (région CH_3) et des septuplets à 3,13 et 3,65 ppm. Des mesures de type COSY nous ont permis de prouver que les signaux à 0,63 et 3,13 ppm d'une part et à 0,98 et 3,65 ppm d'autre part sont corrélés. Cette observation signifie qu'ils appartiennent à deux systèmes de spins différents, avec le motif isopropyle. Des mesures HSQC ont permis de corréler les ^{13}C associés à ces protons et les valeurs obtenues sont présentées dans le Tableau 3.

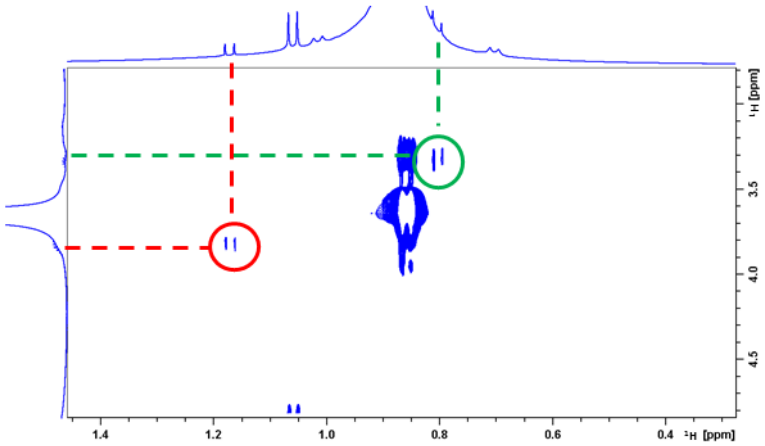


Figure 9: Spectre 2D ^{1}H-COSY d'une solution chauffée 24h à 100°C contenant initialement 10 mg d'UCl_4, 30 mg d'acide benzoïque et 1 mL de solvant isopropanol. Sonde BBO 10 mm.

N'ayant pas assez d'informations pour déterminer la nature de ces deux systèmes de spins, nous avons réfléchi à des espèces chimiques possédant une fonction isopropyle et qui pourrait se former en solution à partir des autres réactifs. Nous avons alors utilisé la

base de données SBDS (*Spectral Database for Organic Compounds*) afin de comparer les spectres ^{1}H et ^{13}C référencés à ceux que nous avons obtenus. Les deux espèces recherchées semblent alors être l'éther di-isopropyle et le chlorure d'isopropyle. Les spectres ^{13}C sont très proches Les données proton diffèrent davantage car le solvant deutéré est différent (chloroforme ou benzène) et les conditions de mesure sont très différentes (acidité notamment). Le Tableau 3 permet de comparer les déplacements chimiques que nous avons mesurés avec ceux de la base de données pour ces deux espèces.

*Tableau 3 : Comparaison des déplacements chimiques ^{1}H et ^{13}C entre les valeurs mesurées et celles issues de la base de données SBDS. Les valeurs de la base de données ont été mesurées dans le chloroforme deutéré sauf les valeurs notées avec * qui ont été mesurées dans du benzène deutéré.*

		Ether di-isopropyle		Chlorure d'isopropyle	
		Exp	SDBS n° 2837	Exp	SDBS n° 2464
^{1}H	CH_3	0,63	1,13	0,98	1,14 *
	CH	3,14	3,64	3,63	3,73 *
^{13}C	CH_3	22,0	22,90	27,2	27,33
	CH	68,8	68,39	53,1	53,84

II. Données cristallographiques

II.1 Th-trim-I

Table 1 Crystal data and structure refinement for Th-trim-I.	
Identification code	Th-trim-I
Empirical formula	$C_{27}H_9O_{23.5}Th_3$
Formula weight	1405.46
Temperature/K	299.28
Crystal system	hexagonal
Space group	$P6_3/m$
a/Å	18.4448(6)
b/Å	18.4448(6)
c/Å	9.8084(3)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	2889.9(2)
Z	2
ρ_{calc}g/cm^3	1.615
μ/mm^{-1}	7.757
F(000)	1258.0
Crystal size/mm^3	0.264 × 0.074 × 0.025
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.55 to 63.128
Index ranges	$-20 \le h \le 27$, $-25 \le k \le 22$, $-14 \le l \le 13$
Reflections collected	46953
Independent reflections	3379 [R_{int} = 0.0522, R_{sigma} = 0.0533]
Data/restraints/parameters	3379/0/93
Goodness-of-fit on F^2	1.127
Final R indexes [I>=2σ (I)]	R_1 = 0.0370, wR_2 = 0.1073
Final R indexes [all data]	R_1 = 0.0649, wR_2 = 0.1178
Largest diff. peak/hole / e Å^{-3}	1.90/-1.21

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-trim-I. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	6461.7(2)	2020.1(2)	2500	18.13(11)
O61	5686(4)	623(3)	3610(4)	46.2(14)
O1	6667	3333	2500	21(2)
O1W	7476(5)	1572(5)	2500	54(2)
O31	6878(3)	2262(3)	4956(4)	33.1(10)
O32	5329(2)	2061(3)	3859(4)	27.5(10)
C3	7594(4)	2892(4)	4955(5)	21.9(11)

C5	5232(5)	-676(5)	2500	23.1(17)
C6	5538(6)	228(5)	2500	25.1(18)
C2	8052(4)	3204(4)	6271(5)	19.9(11)
C1	7633(5)	2899(6)	7500	22.0(17)
C4	5086(4)	-1109(4)	3733(5)	23.3(12)
O2W	7010(30)	540(30)	7500	280(40)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Th-trim-I. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	25.58(18)	18.70(17)	9.60(14)	0	0	10.69(13)
O61	79(4)	24(2)	23(2)	-0.5(18)	16(2)	17(3)
O1	21(3)	21(3)	21(4)	0	0	10.5(16)
O1W	53(5)	50(5)	71(5)	0	0	34(4)
O31	28(2)	40(3)	18.8(19)	-5.0(18)	-7.4(18)	8(2)
O32	29(2)	40(3)	9.6(17)	-0.5(16)	1.8(14)	15(2)
C3	27(3)	30(3)	13(2)	-2(2)	-3(2)	17(3)
C5	29(5)	25(4)	18(3)	0	0	16(4)
C6	27(5)	21(4)	26(4)	0	0	10(4)
C2	23(3)	27(3)	11(2)	0.6(19)	-0.2(19)	14(3)
C1	21(4)	28(4)	12(3)	0	0	8(4)
C4	28(3)	24(3)	15(2)	-3(2)	0(2)	11(3)
O2W	170(40)	120(30)	570(110)	0	0	80(30)

Table 4 Bond Lengths for Th-trim-I.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	O61	2.487(5)		O1	$Th1^4$	2.2571(3)
Th1	$O61^1$	2.487(5)		O31	C3	1.250(7)
Th1	O1	2.2571(3)		O32	$Th1^4$	2.869(4)
Th1	O1W	2.394(8)		O32	$C3^4$	1.265(7)
Th1	O31	2.500(4)		C3	$O32^3$	1.265(7)
Th1	$O31^1$	2.500(4)		C3	C2	1.491(7)
Th1	$O32^1$	2.511(4)		C5	C6	1.469(12)
Th1	$O32^2$	2.869(4)		C5	$C4^1$	1.399(7)
Th1	$O32^3$	2.869(4)		C5	C4	1.399(7)
Th1	O32	2.511(4)		C6	$O61^1$	1.261(6)
Th1	C3	3.064(5)		C2	C1	1.390(6)
Th1	C6	2.863(9)		C2	$C4^5$	1.381(8)
O61	C6	1.261(6)		C1	$C2^6$	1.390(7)
O1	$Th1^3$	2.2571(3)		C4	$C2^7$	1.381(8)

[1]+X,+Y,1/2-Z; [2]1-Y,+X-Y,1/2-Z; [3]1-Y,+X-Y,+Z; [4]1+Y-X,1-X,+Z; [5]1+Y,1-X+Y,1-Z; [6]+X,+Y,3/2-Z; [7]-Y+X,-1+X,1-Z

II.2 Th-btc-II

Table 1 Crystal data and structure refinement forTh-btc-II.	
Identification code	Th-trim-II
Empirical formula	ThOCHN
Formula weight	1335.68
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	20.5158(10)
b/Å	10.0012(5)
c/Å	21.5145(9)
α/°	90
β/°	99.156(2)
γ/°	90
Volume/Å^3	4358.2(4)
Z	0
ρ_{calc}g/cm^3	2.036
μ/mm^{-1}	6.903
F(000)	2508.0
Crystal size/mm^3	0.112 × 0.078 × 0.053
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.01 to 56.64
Index ranges	-27 ≤ h ≤ 27, -13 ≤ k ≤ 13, -28 ≤ l ≤ 28
Reflections collected	64898
Independent reflections	10823 [R_{int} = 0.0881, R_{sigma} = 0.0690]
Data/restraints/parameters	10823/0/474
Goodness-of-fit on F^2	1.024
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1016
Final R indexes [all data]	R_1 = 0.0836, wR_2 = 0.1174
Largest diff. peak/hole / e Å^{-3}	3.22/-2.12

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) forTh-btc-II. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	1481.3(2)	6952.8(3)	4157.6(2)	14.30(8)
Th2	3595.2(2)	7034.7(3)	6012.1(2)	16.20(8)
O71B	2644(3)	7110(8)	4217(3)	33.4(17)
O71A	1652(3)	6172(7)	5215(3)	27.7(15)
O82A	1095(4)	8847(7)	3407(3)	35.2(17)
O72A	2466(3)	6412(9)	6015(3)	41(2)
O91A	532(3)	6160(8)	3345(3)	39.5(19)
O81C	3538(4)	4727(7)	6010(3)	37.1(18)
C6C	2205(5)	11487(9)	4553(4)	25(2)
O81A	1726(3)	7350(7)	3072(3)	31.5(17)
C2C	2858(4)	11464(9)	5587(5)	26(2)

O71C	1890(3)	8838(6)	4786(3)	32.1(16)
O72C	2855(4)	8657(7)	5436(3)	41(2)
O72B	3480(3)	6471(7)	4921(3)	35.3(17)
C1A	1404(4)	6048(9)	6242(4)	18.3(17)
O91C	1879(4)	4844(7)	3967(3)	40.8(19)
O82B	3640(4)	8894(7)	6714(3)	39.5(18)
C5C	2274(5)	2870(9)	4527(4)	26(2)
C7B	3188(4)	6543(9)	4370(4)	21.2(19)
C1C	2494(4)	10790(9)	5085(4)	23.9(19)
O91B	4667(3)	6100(8)	5726(3)	38.9(19)
O92A	559(4)	5306(8)	4289(3)	44(2)
O92B	4667(3)	6552(8)	6721(3)	34.3(17)
C7A	1872(4)	6237(9)	5793(4)	20.6(18)
C6A	782(4)	5468(9)	6039(4)	22.5(19)
O82C	3474(6)	2941(9)	6610(4)	88(4)
C6B	4119(4)	5263(9)	4025(4)	22.9(19)
O92C	1778(7)	2948(9)	3464(4)	96(4)
C3C	2931(5)	12843(9)	5564(4)	26(2)
C2A	1583(4)	6435(9)	6867(4)	23(2)
O81B	2600(5)	9244(11)	6949(4)	72(3)
C5B	4427(4)	4723(10)	3549(4)	26(2)
C5A	377(4)	5179(10)	6484(4)	26(2)
C4B	4158(5)	10048(11)	7920(4)	34(2)
C8A	1336(4)	8347(10)	2969(4)	22(2)
C7C	2418(4)	9323(9)	5108(4)	23(2)
C3A	1159(4)	6174(10)	7301(4)	25(2)
C2B	3230(5)	8908(12)	8246(4)	40(3)
C1B	3522(4)	5927(10)	3870(4)	24.1(19)
C4C	2640(5)	3546(10)	5038(4)	32(2)
C3B	3554(6)	9402(12)	7766(5)	45(3)
C4A	566(5)	5494(10)	7110(4)	28(2)
C9C	1950(6)	3585(10)	3941(5)	37(3)
C9A	270(4)	5470(10)	3729(4)	27(2)
C8B	3236(6)	9149(14)	7095(5)	51(4)
C8C	3336(6)	3548(11)	6115(5)	40(3)
C9B	4940(4)	6010(10)	6292(4)	26(2)
O1SB	548(3)	8058(5)	4555(2)	40.2(17)
C2SB	422(2)	8299(6)	5077(2)	45(3)
N3SB	-188(3)	8251(5)	5252(3)	50(3)
C5SB	-764(2)	7887(11)	4799(4)	88(5)
C4SB	-288(4)	8557(7)	5889(3)	65(4)
N1N	1702(6)	4005(12)	2286(5)	87(4)
O1SA	3425(3)	6313(6)	7136(3)	51(2)
C2SA	3670(3)	5318(6)	7401(3)	54(3)
N3SA	3467(3)	4698(6)	7901(3)	62(3)
C4SA	2910(5)	5216(9)	8168(4)	89(5)
C5SA	3794(5)	3511(9)	8185(5)	112(7)
C42S	4799(11)	12280(17)	5531(10)	89(14)

C22S	4514(8)	9981(14)	5865(7)	71(12)
C52S	4123(11)	11010(18)	4714(8)	99(16)
O1S	4276(4)	8862(9)	5662(4)	61(2)
C21S	4258(6)	9880(10)	5350(4)	108(13)
N3S	4537(5)	11074(9)	5547(6)	102(5)
C41S	4897(13)	11224(14)	6183(7)	104(12)
C51S	4488(11)	12234(11)	5138(9)	91(11)
C3N	1056(10)	4540(20)	2081(9)	109(7)
C2N	1875(12)	2770(20)	1939(11)	133(8)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) forTh-btc-II. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	14.79(15)	17.40(16)	10.05(14)	-1.06(12)	-0.05(10)	-2.41(13)
Th2	15.09(15)	14.98(16)	18.60(16)	-1.75(12)	2.87(11)	0.35(13)
O71B	18(3)	56(5)	26(3)	-3(3)	4(3)	9(3)
O71A	31(4)	41(4)	11(3)	1(3)	3(3)	-9(3)
O82A	54(5)	39(4)	15(3)	4(3)	9(3)	14(4)
O72A	24(4)	74(6)	25(4)	-3(4)	4(3)	-14(4)
O91A	32(4)	61(5)	23(3)	6(3)	-3(3)	-30(4)
O81C	57(5)	17(4)	34(4)	-6(3)	-4(3)	-10(3)
C6C	35(5)	21(5)	18(4)	4(4)	-1(4)	-2(4)
O81A	23(3)	49(5)	23(3)	15(3)	9(3)	17(3)
C2C	23(5)	17(5)	33(5)	4(4)	-9(4)	-4(4)
O71C	31(4)	16(3)	46(4)	-3(3)	-6(3)	2(3)
O72C	57(5)	21(4)	33(4)	-3(3)	-28(3)	12(3)
O72B	38(4)	49(5)	17(3)	-2(3)	-2(3)	18(3)
C1A	18(4)	21(4)	16(4)	-3(3)	2(3)	-3(4)
O91C	67(5)	27(4)	26(4)	6(3)	1(3)	10(4)
O82B	63(5)	31(4)	24(4)	-11(3)	7(3)	-2(4)
C5C	34(5)	21(5)	21(4)	1(4)	-1(4)	-1(4)
C7B	17(4)	29(5)	17(4)	0(4)	2(3)	3(4)
C1C	26(5)	15(4)	29(5)	0(4)	-2(4)	3(4)
O91B	28(4)	64(5)	23(3)	6(3)	-2(3)	21(4)
O92A	39(4)	66(6)	23(4)	6(4)	-5(3)	-26(4)
O92B	25(4)	51(5)	25(4)	-4(3)	0(3)	17(3)
C7A	22(4)	20(5)	19(4)	-2(3)	1(3)	-8(4)
C6A	20(4)	30(5)	16(4)	-8(4)	-1(3)	-9(4)
O82C	153(11)	41(5)	49(6)	3(5)	-43(6)	-35(6)
C6B	21(5)	29(5)	18(4)	0(4)	1(3)	10(4)
O92C	201(13)	30(5)	37(5)	-1(4)	-38(6)	-3(7)
C3C	29(5)	16(5)	32(5)	-4(4)	-2(4)	-9(4)
C2A	18(4)	31(5)	17(4)	-9(4)	-2(3)	-4(4)
O81B	65(6)	104(9)	42(5)	-6(5)	-5(5)	-30(6)
C5B	24(5)	31(5)	25(5)	6(4)	4(4)	11(4)
C5A	18(4)	38(6)	21(5)	-2(4)	0(4)	-13(4)

C4B	43(6)	40(6)	19(5)	-5(4)	9(4)	-26(5)
C8A	14(4)	35(6)	16(4)	6(4)	0(3)	3(4)
C7C	28(5)	21(5)	17(4)	2(3)	-8(4)	0(4)
C3A	27(5)	33(6)	14(4)	-9(4)	2(4)	-3(4)
C2B	39(6)	59(8)	21(5)	-1(5)	-1(4)	-29(6)
C1B	19(4)	31(5)	20(4)	0(4)	-3(3)	4(4)
C4C	42(6)	20(5)	34(6)	8(4)	2(5)	0(4)
C3B	55(7)	62(8)	19(5)	-15(5)	4(5)	-39(6)
C4A	30(5)	38(6)	18(4)	-6(4)	5(4)	-11(4)
C9C	61(8)	19(5)	27(5)	-4(4)	-1(5)	1(5)
C9A	22(5)	37(6)	21(5)	-5(4)	2(4)	-18(4)
C8B	58(8)	73(9)	21(5)	-2(6)	1(5)	-43(7)
C8C	53(7)	28(6)	33(6)	3(5)	-13(5)	-8(5)
C9B	18(4)	37(6)	24(5)	2(4)	3(4)	6(4)

Table 4 Bond Lengths forTh-btc-II.

Atom	Atom	Length/Å		Atom	Atom	Length/Å		Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	O71B	2.373(6)		O82C	C8C	1.220(13)		O91A	C9A	1.262(10)		O1SB	C2SB	1.2160
Th1	O71A	2.378(6)		C6B	C5B	1.395(12)		O81C	C8C	1.281(12)		C2SB	N3SB	1.3633
Th1	O82A	2.533(7)		C6B	C1B	1.386(12)		C6C	C5C[1]	1.392(13)		N3SB	C5SB	1.4527
Th1	O91A	2.529(6)		O92C	C9C	1.212(12)		C6C	C1C	1.391(12)		N3SB	C4SB	1.4506
Th1	O81A	2.498(6)		C3C	C4C[1]	1.385(13)		O81A	C8A	1.275(11)		N1N	C3N	1.43(2)
Th1	O71C	2.392(6)		C3C	C8C[1]	1.510(13)		C2C	C1C	1.387(12)		N1N	C2N	1.51(2)
Th1	O91C	2.321(7)		C2A	C3A	1.398(12)		C2C	C3C	1.388(12)		O1SA	C2SA	1.2163
Th1	O92A	2.558(7)		O81B	C8B	1.296(15)		O71C	C7C	1.285(10)		C2SA	N3SA	1.3619
Th1	C8A	2.887(8)		C5B	C4B[3]	1.396(12)		O72C	C7C	1.243(10)		N3SA	C4SA	1.4532
Th1	C9A	2.915(8)		C5B	C9B[4]	1.483(12)		O72B	C7B	1.242(10)		N3SA	C5SA	1.4496
Th1	O1SB	2.478(5)		C5A	C4A	1.378(12)		C1A	C7A	1.478(11)		C42S	N3S	1.323(14)
Th2	O72A	2.399(7)		C5A	C9A[5]	1.483(11)		C1A	C6A	1.407(11)		C42S	C41S	1.741(19)
Th2	O81C	2.311(7)		C4B	C5B[6]	1.396(12)		C1A	C2A	1.391(11)		C42S	C51S	0.98(3)
Th2	O72C	2.424(6)		C4B	C3B	1.390(13)		O91C	C9C	1.270(12)		C22S	O1S	1.271(16)
Th2	O72B	2.389(6)		C8A	C3A[3]	1.503(11)		O82B	C8B	1.280(14)		C22S	C21S	1.153(17)
Th2	O82B	2.388(7)		C3A	C8A[6]	1.503(11)		C5C	C6C[2]	1.392(13)		C22S	N3S	1.294(12)
Th2	O91B	2.553(6)		C3A	C4A	1.398(12)		C5C	C4C	1.402(13)		C22S	C41S	1.567(17)
Th2	O92B	2.515(6)		C2B	C1B[6]	1.390(12)		C5C	C9C	1.507(13)		C52S	C21S	1.763(12)
Th2	C9B	2.914(9)		C2B	C3B	1.403(14)		C7B	C1B	1.497(12)		C52S	N3S	1.86(2)
Th2	O1SA	2.599(6)		C1B	C2B[3]	1.390(12)		C1C	C7C	1.477(12)		C52S	C51S	1.64(3)
Th2	O1S	2.489(8)		C4C	C3C[2]	1.385(13)		O91B	C9B	1.261(11)		O1S	C21S	1.2164
O71B	C7B	1.249(10)		C3B	C8B	1.508(14)		O92A	C9A	1.266(11)		C21S	N3S	1.3625
O71A	C7A	1.254(10)		C9A	C5A[5]	1.483(11)		O92B	C9B	1.273(11)		N3S	C41S	1.4536
O82A	C8A	1.238(10)		C8C	C3C[2]	1.510(13)		C6A	C5A	1.394(12)		N3S	C51S	1.4500
O72A	C7A	1.250(10)		C9B	C5B[4]	1.483(12)								

[1]+X,1+Y,+Z; [2]+X,-1+Y,+Z; [3]+X,3/2-Y,-1/2+Z; [4]1-X,1-Y,1-Z; [5]-X,1-Y,1-Z; [6]+X,3/2-Y,1/2+Z

II.3 Th-btc-III

Table 1 Crystal data and structure refinement forTh-btc-III.	
Identification code	Th-btc-III
Empirical formula	$C_{35}H_{10}N_3O_{20}Th_2$
Formula weight	1256.54
Temperature/K	296(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	20.2327(14)
b/Å	10.0714(7)
c/Å	21.6730(14)
α/°	90
β/°	97.856(3)
γ/°	90
Volume/Å^3	4374.9(5)
Z	4
ρ_{calc}g/cm^3	1.908
μ/mm^{-1}	6.868
F(000)	2324.0
Crystal size/mm^3	0.1 × 0.084 × 0.042
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.032 to 61.066
Index ranges	-26 ≤ h ≤ 28, -14 ≤ k ≤ 14, -25 ≤ l ≤ 30
Reflections collected	195654
Independent reflections	13327 [R_{int} = 0.0611, R_{sigma} = 0.0364]
Data/restraints/parameters	13327/0/488
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0377, wR_2 = 0.0919
Final R indexes [all data]	R_1 = 0.0645, wR_2 = 0.1022
Largest diff. peak/hole / e Å^{-3}	2.23/-1.35

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) forTh-btc-III. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	1489.6(2)	7905.7(2)	4130.6(2)	14.17(5)
Th2	3564.8(2)	7855.6(2)	5930.4(2)	15.14(5)
O71B	1615(2)	8651(5)	5182.7(17)	28.5(10)
O91B	1761(2)	7475(5)	3052.3(18)	29(1)
O71A	3441(2)	8522(5)	4874.2(18)	35.0(11)
O92B	1067(3)	6050(5)	3378.2(18)	35.0(11)
O92A	3276(3)	7578(6)	7000(2)	49.4(15)
O72A	2682(2)	7719(5)	4149(2)	35.5(11)
O91A	3839(3)	5955(5)	6674.3(19)	40.3(12)
O71C	1925(2)	6014(4)	4740(2)	33.7(11)
O81A	4592(2)	8476(5)	6693(2)	39.8(12)

O82B	557(2)	8777(5)	3330.9(19)	37.6(12)
O7	1925(3)	9989(5)	3984(2)	39.9(12)
O21D	565(3)	6793(5)	4531(2)	43.7(12)
O81B	569(2)	9562(6)	4277(2)	41.7(13)
C6B	1564(3)	8576(6)	6843(2)	21.5(12)
C1B	1371(3)	8908(6)	6218(2)	20.3(11)
C1A	3607(3)	8861(6)	3835(2)	23.2(12)
C2B	751(3)	9502(6)	6031(2)	22.3(12)
C7A	3214(3)	8339(6)	4319(2)	21.7(12)
C2A	4164(3)	9644(7)	4001(3)	27.8(13)
C5B	1150(3)	8884(6)	7283(2)	20.8(11)
C9B	1339(3)	6545(6)	2944(2)	20.2(11)
C3B	355(3)	9858(6)	6476(3)	25.1(13)
C9A	3627(3)	6524(7)	7104(3)	30.7(14)
C4B	561(3)	9570(7)	7102(3)	26.5(13)
C3C	2891(4)	1992(6)	5560(3)	32.8(15)
C5A	3783(3)	6029(7)	7760(3)	32.9(15)
C7B	1832(3)	8634(6)	5752(2)	23.3(12)
C1C	2480(3)	4052(6)	5069(3)	25.5(13)
C6A	3414(3)	8520(7)	3213(3)	30.8(15)
C6C	2198(3)	3358(6)	4547(3)	27.9(13)
C3A	4517(3)	10139(7)	3542(3)	29.7(14)
C5C	2250(3)	1966(6)	4528(3)	30.2(14)
C2C	2832(3)	3380(6)	5574(3)	30.4(15)
O82A	4646(3)	8907(7)	5714(2)	59.0(18)
O72B	2426(2)	8431(7)	5962(2)	56.9(18)
O81C	3464(3)	10128(5)	6042(3)	60.4(18)
O72C	2834(3)	6163(5)	5442(3)	54.5(17)
C8B	296(3)	9464(7)	3723(3)	29.3(14)
C7C	2414(3)	5521(6)	5089(3)	27.8(14)
C4C	2605(4)	1309(7)	5037(3)	35.2(16)
C4A	4323(3)	9812(7)	2921(3)	33.0(15)
C9C	1933(4)	11246(7)	3961(3)	41.1(18)
C8A	4877(3)	9017(8)	6279(3)	34.8(16)
C8C	3266(5)	11305(7)	6114(4)	54(2)
C21D	459(5)	6570(10)	5091(4)	59(2)
C13D	4411(8)	4942(19)	5631(8)	135(6)
O20C	1674(6)	11877(6)	3519(3)	119(4)
N2D	-152(4)	6760(9)	5273(4)	68(2)
O82C	3395(6)	11909(7)	6601(3)	137(5)
N1D	4414(6)	3876(13)	5303(5)	100(3)
O11D	4227(3)	6161(7)	5474(3)	69.1(18)
C23D	-268(7)	6434(15)	5903(7)	107(4)
C22D	-738(8)	7214(16)	4827(7)	118(5)
C12D	4723(9)	2630(20)	5464(9)	140(6)
C11D	4101(11)	3850(20)	4619(10)	174(8)
N1S	3453(13)	4240(30)	2864(11)	115(8)
N2S	1655(9)	1195(19)	2235(8)	74(5)

C12S	2917(11)	4830(20)	3056(10)	73(6)
C11S	4063(14)	4690(30)	2877(13)	99(8)
C21S	2013(16)	200(30)	2100(14)	117(10)
C22S	1060(20)	900(40)	2150(18)	156(14)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) forTh-btc-III. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Th1	15.30(9)	16.04(10)	10.53(8)	-0.74(7)	-0.49(7)	2.50(7)
Th2	15.7(1)	15.31(10)	14.10(8)	0.24(7)	0.94(7)	-0.78(7)
O71B	36(2)	34(2)	14.2(17)	-4.7(17)	-0.5(17)	11(2)
O91B	26(2)	43(3)	19.1(18)	-15.2(18)	5.2(17)	-16(2)
O71A	39(3)	52(3)	12.3(17)	2.2(19)	-0.8(18)	-17(2)
O92B	56(3)	34(3)	15.6(18)	-4.5(17)	5(2)	-15(2)
O92A	49(3)	72(4)	29(2)	21(3)	12(2)	33(3)
O72A	21(2)	60(3)	26(2)	-1(2)	1.2(18)	-10(2)
O91A	74(4)	28(2)	18(2)	3.0(18)	4(2)	7(2)
O71C	41(3)	17(2)	38(2)	4.4(18)	-12(2)	4.3(19)
O81A	36(3)	56(3)	26(2)	6(2)	-3(2)	-24(2)
O82B	38(3)	50(3)	22(2)	-3(2)	-0.9(19)	26(2)
O7	59(3)	23(2)	37(3)	-7(2)	5(2)	-10(2)
O81B	39(3)	61(3)	23(2)	-2(2)	-4(2)	28(3)
C6B	20(3)	29(3)	14(2)	8(2)	-1(2)	5(2)
C1B	19(3)	29(3)	13(2)	1(2)	0(2)	4(2)
C1A	24(3)	31(3)	14(2)	-3(2)	0(2)	-7(2)
C2B	21(3)	28(3)	17(2)	4(2)	-2(2)	5(2)
C7A	19(3)	30(3)	16(2)	-3(2)	2(2)	-1(2)
C2A	27(3)	39(4)	17(2)	-6(2)	1(2)	-11(3)
C5B	20(3)	27(3)	15(2)	7(2)	1(2)	4(2)
C9B	17(3)	27(3)	16(2)	-6(2)	-1(2)	0(2)
C3B	23(3)	29(3)	22(3)	5(2)	1(2)	13(2)
C9A	28(3)	39(4)	25(3)	8(3)	2(3)	4(3)
C4B	24(3)	40(4)	15(2)	4(2)	3(2)	9(3)
C3C	47(4)	16(3)	33(3)	2(2)	-6(3)	6(3)
C5A	34(3)	46(4)	18(3)	8(3)	0(2)	15(3)
C7B	22(3)	31(3)	16(2)	2(2)	-1(2)	9(2)
C1C	25(3)	15(3)	33(3)	1(2)	-7(3)	-3(2)
C6A	29(3)	45(4)	19(3)	-5(3)	2(2)	-14(3)
C6C	32(3)	17(3)	32(3)	4(2)	-6(3)	-2(2)
C3A	28(3)	40(4)	20(3)	-5(3)	-3(2)	-15(3)
C5C	40(4)	19(3)	29(3)	-2(2)	-5(3)	-1(3)
C2C	39(4)	17(3)	30(3)	-1(2)	-11(3)	4(3)
O82A	47(3)	105(5)	24(2)	-12(3)	1(2)	-47(3)
O72B	27(3)	119(6)	24(2)	10(3)	3(2)	32(3)
O81C	100(5)	22(3)	49(3)	0(2)	-26(3)	20(3)
O72C	67(4)	22(2)	61(3)	4(2)	-41(3)	-13(2)

C8B	25(3)	38(4)	23(3)	2(3)	-3(2)	17(3)
C7C	32(3)	16(3)	32(3)	0(2)	-10(3)	0(2)
C4C	51(4)	18(3)	34(3)	2(3)	-4(3)	0(3)
C4A	37(4)	43(4)	18(3)	-4(3)	5(3)	-19(3)
C9C	65(5)	19(3)	34(3)	-6(3)	-12(3)	0(3)
C8A	29(3)	47(4)	26(3)	-6(3)	-1(3)	-13(3)
C8C	92(7)	23(4)	38(4)	3(3)	-18(4)	8(4)
O20C	228(11)	28(3)	71(5)	-6(3)	-84(6)	9(5)
O82C	283(14)	48(4)	54(4)	-17(3)	-68(6)	66(6)

Table 4 Bond Lengths forTh-btc-III.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Th1	O7	2.314(5)	C2A	C3A	1.393(9)	O71B	C7B	1.252(6)	O82A	C8A	1.256(7)
Th1	O71B	2.381(4)	C5B	C4B	1.385(8)	O91B	C9B	1.269(7)	O81C	C8C	1.268(9)
Th1	O72A	2.415(4)	C5B	C9B[1]	1.494(7)	O71A	C7A	1.241(6)	O72C	C7C	1.245(7)
Th1	O71C	2.415(4)	C9B	C5B[2]	1.494(7)	O92B	C9B	1.256(7)	C8B	C3B[3]	1.495(8)
Th1	O21D	2.439(5)	C3B	C4B	1.394(7)	O92A	C9A	1.280(8)	C4A	C5A[2]	1.390(8)
Th1	O91B	2.511(4)	C3B	C8B[3]	1.495(8)	O72A	C7A	1.255(7)	C9C	O20C	1.208(9)
Th1	O82B	2.538(4)	C9A	C5A	1.498(8)	O91A	C9A	1.220(8)	C9C	C5C[6]	1.495(8)
Th1	O92B	2.550(4)	C3C	C4C	1.383(9)	O71C	C7C	1.261(7)	C8A	C3A[5]	1.499(8)
Th1	O81B	2.553(5)	C3C	C2C	1.403(8)	O81A	C8A	1.254(8)	C8C	O82C	1.214(10)
Th1	C9B	2.894(5)	C3C	C8C[4]	1.500(9)	O82B	C8B	1.265(7)	C8C	C3C[6]	1.500(9)
Th1	C8B	2.913(6)	C5A	C6A[1]	1.389(9)	O7	C9C	1.268(8)	C21D	N2D	1.360(12)
Th2	O81C	2.313(5)	C5A	C4A[1]	1.389(8)	O21D	C21D	1.281(10)	C13D	N1D	1.289(19)
Th2	O71A	2.366(4)	C7B	O72B	1.242(7)	O81B	C8B	1.255(7)	C13D	O11D	1.313(18)
Th2	O72B	2.386(5)	C1C	C6C	1.384(8)	C6B	C5B	1.389(8)	N2D	C23D	1.454(16)
Th2	O72C	2.405(5)	C1C	C2C	1.397(8)	C6B	C1B	1.397(7)	N2D	C22D	1.496(17)
Th2	O11D	2.459(7)	C1C	C7C	1.486(8)	C1B	C2B	1.398(7)	N1D	C12D	1.42(2)
Th2	O92A	2.483(5)	C6A	C5A[2]	1.389(9)	C1B	C7B	1.491(8)	N1D	C11D	1.53(2)
Th2	O91A	2.515(4)	C6C	C5C	1.406(8)	C1A	C2A	1.384(8)	N1S	C11S	1.31(3)
Th2	O82A	2.532(5)	C3A	C4A	1.389(8)	C1A	C6A	1.393(7)	N1S	C12S	1.35(3)
Th2	O81A	2.550(4)	C3A	C8A[5]	1.499(8)	C1A	C7A	1.496(8)	N2S	C22S	1.22(4)
Th2	C9A	2.864(6)	C5C	C4C	1.398(8)	C2B	C3B	1.384(8)	N2S	C21S	1.29(3)
Th2	C8A	2.905(6)	C5C	C9C[4]	1.495(8)						

[1]+X,3/2-Y,1/2+Z; [2]+X,3/2-Y,-1/2+Z; [3]-X,2-Y,1-Z; [4]+X,-1+Y,+Z; [5]1-X,2-Y,1-Z; [6]+X,1+Y,+Z

II.4 Th-btc-IV

Table 1 Crystal data and structure refinement for Th-btc-IV.	
Identification code	Th-btc-IV
Empirical formula	$C_{15}H_3N_3O_{11}Th$
Formula weight	633.24
Temperature/K	299.56
Crystal system	orthorhombic
Space group	Pccn
a/Å	19.4800(8)
b/Å	21.5673(8)
c/Å	11.1237(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4673.4(3)
Z	8
ρ_{calc}g/cm^3	1.800
μ/mm^{-1}	6.435
F(000)	2336.0
Crystal size/mm^3	0.246 × 0.214 × 0.074
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.818 to 52.816
Index ranges	-24 ≤ h ≤ 24, -26 ≤ k ≤ 26, -13 ≤ l ≤ 13
Reflections collected	77227
Independent reflections	4784 [R_{int} = 0.0294, R_{sigma} = 0.0116]
Data/restraints/parameters	4784/0/271
Goodness-of-fit on F^2	1.364
Final R indexes [I>=2σ (I)]	R_1 = 0.0588, wR_2 = 0.1633
Final R indexes [all data]	R_1 = 0.0642, wR_2 = 0.1659
Largest diff. peak/hole / e Å^{-3}	3.34/-2.72

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-btc-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	4926.1(3)	1059.5(2)	6435.9(4)	31.54(17)
O1NA	3711(7)	711(6)	5730(13)	73(4)
O71A	4900(6)	872(4)	4328(8)	48(3)
O1SA	4132(7)	1048(5)	8115(12)	62(3)
O2NA	3915(8)	1689(5)	5619(12)	67(4)
O91A	5608(6)	958(4)	8106(9)	50(3)
O82A	5409(6)	2029(4)	5479(8)	47(3)
O72A	4827(6)	-18(4)	6638(9)	50(3)
O92A	6001(6)	150(4)	9124(9)	52(3)
O4NA	2971(10)	1328(11)	4920(30)	164(11)
O1SB	6058(7)	765(6)	5761(11)	61(3)

O81A	4989(6)	2125(4)	7300(9)	50(3)
N3SA	3665(7)	1594(7)	9606(13)	56(4)
N3NA	3512(10)	1244(9)	5390(20)	86(6)
N3SB	7131(10)	391(11)	5950(20)	105(7)
C2SB	6493(11)	419(10)	6243(18)	67(5)
C7A	5115(7)	591(5)	3413(10)	32(3)
C4SA	3511(12)	1641(12)	10903(17)	88(7)
C5SB	7310(30)	740(30)	4760(70)	340(50)
C1A	5282(7)	963(5)	2363(10)	28(3)
C2A	5226(7)	1608(5)	2350(11)	31(3)
C6A	5485(7)	671(5)	1283(10)	28(3)
C8A	5249(7)	2363(5)	6357(12)	36(3)
C3A	5341(7)	1949(5)	1303(10)	29(3)
C5SA	3448(14)	2112(9)	8790(20)	93(8)
C4A	5511(7)	1652(5)	241(10)	29(3)
C5A	5590(7)	1016(5)	282(16)	44(4)
C9A	5753(7)	667(6)	9086(11)	34(3)
C2SA	3982(8)	1101(7)	9197(15)	47(4)
C4SB	7626(15)	-21(15)	6610(30)	139(13)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Th-btc-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka*b*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Th1	61.7(3)	9.8(2)	23.2(2)	0.27(15)	8.7(2)	2.31(18)
O1NA	79(9)	66(8)	75(10)	-10(7)	6(7)	-15(7)
O71A	96(8)	17(4)	31(5)	0(4)	2(5)	1(5)
O1SA	83(8)	35(6)	67(8)	-9(5)	29(7)	-4(6)
O2NA	98(10)	39(6)	65(8)	6(6)	-6(7)	19(7)
O91A	95(8)	29(5)	25(5)	3(4)	1(5)	11(5)
O82A	97(8)	11(4)	33(5)	-5(4)	18(5)	-5(5)
O72A	106(9)	10(4)	35(5)	2(4)	8(6)	2(5)
O92A	103(9)	26(5)	26(5)	-7(4)	6(5)	19(5)
O4NA	89(13)	150(19)	250(30)	0(20)	-76(17)	20(13)
O1SB	77(8)	57(7)	50(7)	3(6)	23(6)	15(6)
O81A	101(9)	16(4)	33(5)	-1(4)	17(6)	-2(5)
N3SA	55(8)	59(9)	53(8)	-28(7)	12(7)	-2(7)
N3NA	73(12)	73(12)	112(16)	-3(12)	-12(11)	14(10)
N3SB	67(12)	114(17)	130(20)	-11(15)	15(12)	11(11)
C2SB	72(12)	72(12)	57(12)	-20(10)	4(10)	11(10)
C7A	59(8)	17(5)	21(6)	0(4)	-8(6)	1(5)
C4SA	99(16)	130(20)	39(10)	-42(12)	17(10)	-5(14)
C5SB	200(50)	380(80)	460(100)	260(80)	210(60)	80(50)
C1A	54(8)	11(5)	18(5)	5(4)	2(5)	-9(5)
C2A	53(8)	15(5)	25(6)	-5(4)	-5(6)	3(5)
C6A	51(7)	10(5)	23(6)	7(4)	-4(5)	10(5)
C8A	62(8)	12(5)	33(7)	0(5)	0(6)	-1(5)

C3A	50(7)	19(5)	17(5)	-2(4)	-1(5)	-1(5)
C5SA	130(20)	52(11)	96(18)	-1(12)	27(15)	38(13)
C4A	54(8)	20(6)	14(5)	5(4)	4(5)	1(5)
C5A	47(8)	8(5)	77(11)	7(6)	-28(8)	-1(5)
C9A	59(8)	22(6)	20(6)	-2(5)	1(6)	4(6)
C2SA	50(8)	47(9)	44(9)	-20(7)	16(7)	-7(7)
C4SB	100(20)	140(30)	180(30)	-30(30)	-20(20)	50(20)

Table 4 Bond Lengths for Th-btc-IV.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	O1NA	2.605(14)		O1SB	C2SB	1.25(2)
Th1	O71A	2.381(9)		O81A	C8A	1.273(16)
Th1	O1SA	2.425(12)		N3SA	C4SA	1.48(2)
Th1	O2NA	2.560(12)		N3SA	C5SA	1.50(3)
Th1	O91A	2.294(11)		N3SA	C2SA	1.312(19)
Th1	O82A	2.528(9)		N3SB	C2SB	1.29(3)
Th1	O72A	2.342(8)		N3SB	C5SB	1.56(5)
Th1	O1SB	2.414(12)		N3SB	C4SB	1.50(4)
Th1	O81A	2.494(9)		C7A	O72A[1]	1.243(14)
Th1	N3NA	3.019(19)		C7A	C1A	1.454(15)
Th1	C8A	2.883(11)		C1A	C2A	1.397(14)
O1NA	N3NA	1.27(2)		C1A	C6A	1.412(16)
O71A	C7A	1.256(15)		C2A	C3A	1.395(16)
O1SA	C2SA	1.245(19)		C6A	C5A	1.356(19)
O2NA	N3NA	1.27(2)		C8A	C3A[2]	1.496(15)
O91A	C9A	1.288(15)		C3A	C8A[3]	1.495(15)
O82A	C8A	1.253(15)		C3A	C4A	1.385(16)
O72A	C7A[1]	1.243(14)		C4A	C5A	1.380(15)
O92A	C9A	1.216(15)		C5A	C9A[4]	1.56(2)
O4NA	N3NA	1.19(2)		C9A	C5A[5]	1.56(2)

[1]1-X,-Y,1-Z; [2]+X,1/2-Y,1/2+Z; [3]+X,1/2-Y,-1/2+Z; [4]+X,+Y,-1+Z; [5]+X,+Y,1+Z

II.5 Th-btc-V

Table 1 Crystal data and structure refinement for Th-btc-V.

Identification code	Th-btc-V
Empirical formula	$C_{27}H_9O_{21}Th_{2.25}$
Formula weight	1191.43
Temperature/K	299.39
Crystal system	trigonal
Space group	R-3
a/Å	25.5111(13)
b/Å	25.5111(13)
c/Å	24.095(2)

α/°	90
β/°	90
γ/°	120
Volume/Å^3	13580.4(19)
Z	18
ρ_{calc}g/cm^3	2.622
μ/mm^{-1}	11.167
F(000)	9747.0
Crystal size/mm^3	0.063 × 0.051 × 0.048
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.5 to 46.526
Index ranges	-27 ≤ h ≤ 27, -27 ≤ k ≤ 28, -26 ≤ l ≤ 26
Reflections collected	69213
Independent reflections	4323 [R_{int} = 0.0518, R_{sigma} = 0.0222]
Data/restraints/parameters	4323/0/444
Goodness-of-fit on F^2	1.128
Final R indexes [I>=2σ (I)]	R_1 = 0.0313, wR_2 = 0.0638
Final R indexes [all data]	R_1 = 0.0423, wR_2 = 0.0672
Largest diff. peak/hole / e Å^{-3}	1.91/-0.81

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-btc-V. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th2	8091.5(2)	523.0(2)	9617.9(2)	10.14(10)
Th1	8113.5(2)	504.8(2)	7140.3(2)	11.6(1)
Th3	3333	-3333	10313.1(2)	7.25(15)
O71C	7238(2)	-476(2)	9711(3)	27.0(14)
O72C	8634(2)	1482(2)	10064(2)	23.6(13)
O71A	8311(2)	1156(2)	7916(2)	23.1(13)
O92A	7266(2)	642(3)	9344(2)	22.2(13)
O92B	8033(3)	-67(2)	8843(2)	24.1(13)
O81A	7092(2)	-176(2)	7374(2)	22.8(13)
O72A	8402(3)	1196(2)	8836(2)	29.6(15)
O81B	9107(2)	732(3)	7415(2)	28.5(14)
O91A	7580(2)	182(3)	6281(2)	25.5(14)
O81C	4382(3)	-2986(3)	10411(3)	39.3(17)
O82B	2591(3)	-3534(3)	9601(2)	31.2(15)
O71B	9136(2)	876(3)	9443(2)	26.6(14)
O0AA	8432(2)	-9(2)	10167(2)	22.3(13)
O91B	8044(3)	-96(3)	7925(2)	26.3(14)
O91C	7641(3)	1101(3)	6983(3)	30.5(15)
O72B	7600(2)	449(2)	10491(2)	23.4(13)
O82C	8272(3)	-226(2)	6711(2)	27.4(14)
C8B	9602(4)	743(4)	7442(3)	24(2)
C1B	10023(3)	1252(4)	8919(3)	20.1(19)
C7B	9697(4)	1226(4)	9439(3)	18.3(19)
C3B	9977(4)	1015(4)	7940(3)	22(2)
C5B	8455(4)	-605(4)	8412(3)	19.9(19)

C2B	9689(4)	999(4)	8437(3)	23(2)
O92C	7833(2)	2027(3)	6776(2)	27.1(14)
C6C	6415(3)	616(4)	6704(3)	19.9(19)
C5C	6800(4)	1227(4)	6818(4)	23(2)
C1C	6281(4)	-1262(4)	9981(3)	20.2(19)
C6B	8477(4)	-873(4)	8904(3)	23(2)
C9C	7470(4)	1467(4)	6862(3)	21.0(19)
C1A	9049(4)	2069(4)	8331(3)	20.0(19)
C4B	8712(4)	-684(4)	7930(3)	24(2)
C7A	8558(4)	1429(4)	8367(3)	19.0(19)
C7C	6940(4)	-1019(4)	9872(3)	20.1(19)
C2C	5891(4)	-1885(4)	10024(4)	24(2)
C2A	9470(4)	2330(3)	8762(3)	20.7(19)
C4C	6563(4)	1609(4)	6873(3)	25(2)
C8C	4882(4)	-2778(4)	10175(4)	25(2)
C8A	6527(4)	-495(4)	7452(3)	19.0(19)
C9A	6735(3)	542(3)	9286(3)	16.5(18)
C6A	9085(4)	2427(4)	7878(3)	20.0(19)
C3C	5283(4)	-2110(3)	10141(3)	21.0(19)
C3A	9916(4)	2931(3)	8740(3)	17.6(18)
O1W	3608(4)	-3816(4)	11090(4)	75(3)
C4A	9940(4)	3291(4)	8289(3)	21.8(19)
O2W	7415(8)	1767(8)	8409(7)	207(7)
O3W	7958(7)	2965(7)	8236(6)	159(5)
C5A	6369(4)	178(4)	8801(3)	17.5(18)
C9B	8157(3)	-229(3)	8388(3)	14.9(17)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Th-btc-V. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Th2	8.23(16)	9.41(16)	12.15(16)	1.26(12)	1.39(12)	3.95(13)
Th1	10.06(16)	10.82(16)	14.41(17)	-0.13(12)	-2.12(11)	5.58(12)
Th3	6.3(2)	6.3(2)	9.2(3)	0	0	3.14(10)
O71C	18(3)	7(3)	52(4)	7(3)	5(3)	3(3)
O72C	20(3)	14(3)	35(3)	-6(3)	1(3)	7(3)
O71A	26(3)	13(3)	21(3)	-5(3)	-4(3)	4(3)
O92A	18(3)	32(3)	22(3)	-7(3)	-8(2)	17(3)
O92B	32(4)	27(3)	19(3)	1(3)	4(3)	19(3)
O81A	17(3)	26(3)	21(3)	2(3)	4(2)	8(3)
O72A	36(4)	18(3)	19(3)	4(3)	-2(3)	2(3)
O81B	20(3)	42(4)	31(3)	-9(3)	-13(3)	20(3)
O91A	24(3)	24(3)	20(3)	3(3)	-9(3)	6(3)
O81C	25(4)	28(4)	60(4)	-2(3)	12(3)	9(3)
O82B	27(4)	29(4)	33(4)	5(3)	-3(3)	10(3)
O71B	8(3)	33(4)	31(3)	-1(3)	3(3)	4(3)
O0AA	27(3)	24(3)	19(3)	5(3)	-3(3)	14(3)

O91B	33(4)	34(4)	22(3)	7(3)	2(3)	24(3)
O91C	21(3)	20(3)	58(4)	3(3)	-5(3)	16(3)
O72B	21(3)	26(3)	26(3)	6(3)	12(3)	14(3)
O82C	32(4)	20(3)	35(3)	-7(3)	0(3)	16(3)
C8B	23(5)	24(5)	24(5)	0(4)	7(4)	12(4)
C1B	14(5)	27(5)	17(4)	0(4)	3(4)	9(4)
C7B	22(5)	15(4)	23(5)	-2(4)	-5(4)	13(4)
C3B	14(5)	33(5)	20(4)	-12(4)	-5(4)	13(4)
C5B	22(5)	22(5)	21(4)	3(4)	2(4)	14(4)
C2B	13(4)	29(5)	23(5)	-6(4)	-1(4)	7(4)
O92C	15(3)	22(4)	42(4)	10(3)	3(3)	8(3)
C6C	14(4)	20(5)	30(5)	1(4)	-1(4)	13(4)
C5C	12(4)	21(5)	37(5)	9(4)	6(4)	10(4)
C1C	15(4)	16(5)	29(5)	1(4)	-1(4)	6(4)
C6B	28(5)	25(5)	21(5)	-3(4)	-3(4)	16(4)
C9C	22(5)	15(5)	25(5)	0(4)	1(4)	9(4)
C1A	24(5)	17(5)	13(4)	0(4)	-3(4)	6(4)
C4B	38(5)	25(5)	19(5)	1(4)	-1(4)	22(4)
C7A	25(5)	17(4)	19(5)	2(4)	1(4)	13(4)
C7C	19(5)	20(5)	22(5)	-3(4)	-2(4)	11(4)
C2C	20(5)	24(5)	36(5)	0(4)	0(4)	17(4)
C2A	22(5)	14(5)	19(4)	3(4)	0(4)	4(4)
C4C	23(5)	15(5)	30(5)	-7(4)	-2(4)	4(4)
C8C	20(5)	26(5)	33(5)	1(4)	-3(4)	15(4)
C8A	17(5)	22(5)	13(4)	1(4)	-1(4)	6(4)
C9A	13(5)	16(4)	19(4)	1(4)	-3(4)	6(4)
C6A	16(4)	18(5)	18(4)	3(4)	-3(4)	2(4)
C3C	17(5)	7(4)	34(5)	-2(4)	-1(4)	2(4)
C3A	18(4)	16(4)	16(4)	2(3)	-2(4)	6(4)
O1W	52(5)	78(6)	72(6)	24(5)	-8(4)	16(5)
C4A	28(5)	17(5)	22(4)	0(4)	0(4)	12(4)
C5A	18(5)	23(5)	14(4)	-6(4)	-3(3)	13(4)
C9B	18(4)	10(4)	16(4)	3(3)	1(4)	6(4)

Table 4 Bond Lengths for Th-btc-V.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
Th2	O71C	2.395(5)	Th3	O82B^{3}	2.412(6)	C8B	O82B^{10}	1.264(10)	C1A	C7A	1.483(11)
Th2	O72C	2.381(5)	Th3	O1W	2.524(8)	C8B	C3B	1.474(11)	C1A	C2A	1.400(11)
Th2	O92A	2.367(5)	Th3	O1W^{3}	2.524(8)	C1B	C7B	1.488(11)	C1A	C6A	1.397(11)
Th2	O92B	2.356(5)	Th3	O1W^{2}	2.524(8)	C1B	C2B	1.393(11)	C4B	C3B^{12}	1.388(11)
Th2	O72A	2.402(5)	O71C	C7C	1.262(10)	C1B	C6B^{11}	1.391(11)	C7C	O72C^{7}	1.259(9)
Th2	O71B	2.386(5)	O72C	C7C^{4}	1.259(9)	C7B	O0AA^{4}	1.244(9)	C2C	C3C	1.387(11)
Th2	O0AA	2.351(5)	O71A	C7A	1.274(9)	C3B	C2B	1.395(11)	C2A	C3A	1.381(11)
Th2	O72B	2.406(5)	O92A	C9A	1.254(9)	C3B	C4B^{11}	1.388(11)	C4C	C3C^{5}	1.401(11)
Th1	O71A	2.381(5)	O92B	C9B	1.265(9)	C5B	C6B	1.384(11)	C8C	O82C^{9}	1.258(10)
Th1	O81A	2.367(5)	O81A	C8A	1.265(9)	C5B	C4B	1.397(11)	C8C	C3C	1.489(11)

Th1	O81B	2.393(5)		O72A	C7A	1.245(9)		C5B	C9B	1.494(11)		C8A	O72B[5]	1.244(9)
Th1	O91A	2.387(5)		O81B	C8B	1.252(10)		O92C	Th1[1]	2.402(5)		C8A	C3A[13]	1.504(11)
Th1	O91B	2.384(5)		O91A	C9A[5]	1.255(9)		O92C	C9C	1.273(10)		C9A	O91A[8]	1.255(9)
Th1	O91C	2.397(5)		O81C	C8C	1.246(10)		C6C	C5C	1.391(11)		C9A	C5A	1.493(11)
Th1	O82C	2.336(5)		O82B	C8B[6]	1.264(10)		C6C	C1C[5]	1.402(11)		C6A	C5A[14]	1.390(11)
Th1	O92C[1]	2.402(5)		O71B	C7B	1.251(9)		C5C	C9C	1.505(11)		C3C	C4C[8]	1.401(11)
Th3	O81C[2]	2.372(6)		O0AA	C7B[7]	1.244(9)		C5C	C4C	1.387(11)		C3A	C8A[14]	1.505(11)
Th3	O81C[3]	2.372(6)		O91B	C9B	1.242(9)		C1C	C6C[8]	1.403(11)		C3A	C4A	1.402(11)
Th3	O81C	2.372(6)		O91C	C9C	1.245(9)		C1C	C7C	1.494(11)		C4A	C5A[14]	1.378(11)
Th3	O82B[2]	2.412(6)		O72B	C8A[8]	1.244(9)		C1C	C2C	1.396(11)		C5A	C6A[13]	1.390(11)
Th3	O82B	2.412(6)		O82C	C8C[9]	1.258(10)		C6B	C1B[12]	1.391(11)		C5A	C4A[13]	1.378(11)

[1]5/3-X,1/3-Y,4/3-Z; [2]1+Y-X,-X,+Z; [3]-Y,-1+X-Y,+Z; [4]1+Y,1-X+Y,2-Z; [5]4/3+Y-X,2/3-X,-1/3+Z; [6]-2/3-Y+X,-4/3+X,5/3-Z; [7]-Y+X,-1+X,2-Z; [8]2/3-Y,-2/3+X-Y,1/3+Z; [9]4/3-X,-1/3-Y,5/3-Z; [10]4/3+Y,2/3-X+Y,5/3-Z; [11]2+Y-X,1-X,+Z; [12]1-Y,-1+X-Y,+Z; [13]1/3+Y,2/3-X+Y,5/3-Z; [14]1/3-Y+X,-1/3+X,5/3-Z

II.6 Th-btc-VI

Table 1 Crystal data and structure refinement for Th-btc-VI	
Identification code	Th-btc-VI
Empirical formula	$C_{18}H_6O_{16}Th_2$
Formula weight	942.3
Temperature/K	293
Crystal system	triclinic
Space group	*P*-1
a/Å	5.68460(10)
b/Å	8.9362(2)
c/Å	9.9877(2)
α/°	82.3930(10)
β/°	89.6390(10)
γ/°	87.2530(10)
Volume/Å^3	502.319(18)
Z	1
ρ_{calc}g/cm^3	3.114
μ/mm^{-1}	14.877
F(000)	2725.0
Crystal size/mm^3	0.060 x 0.058 x 0.019
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.877 to 30.368
Index ranges	$-7 \le h \le 7$, $-11 \le k \le 13$, $-12 \le l \le 14$
Reflections collected	8098
Independent reflections	5840 [R_{int} = 0.0288]
Data/restraints/parameters	5840/0/164
Goodness-of-fit on F^2	1.24
Final R indexes [I>=2σ (I)]	R_1 = 0.0293, wR_2 = 0.0322
Final R indexes [all data]	R_1 = 0.0323, wR_2 = 0.0326

Largest diff. peak/hole / e Å^{-3}	1.84/-1.57

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-btc-VI U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	0.02307(4)	0.68058(3)	-0.13237(2)	0.01150(5)
O1h	-0.2366(6)	0.5354(4)	0.0131(4)	0.0140(12)
O1w	-0.2469(7)	0.8807(5)	-0.0547(5)	0.0265(16)
O71a	0.1322(7)	0.7289(5)	0.0934(4)	0.0240(14)
O72a	-0.0746(7)	0.4657(4)	-0.2515(4)	0.0193(14)
O81a	0.3475(7)	0.6270(5)	-0.2762(4)	0.0178(13)
O82a	-0.3154(7)	0.7381(5)	-0.2713(4)	0.0203(14)
O91a	0.2747(6)	0.9156(4)	-0.1317(4)	0.0170(11)
O92a	0.0778(7)	0.9147(5)	-0.3193(4)	0.0260(15)
C1a	0.3304(10)	0.7223(6)	0.3002(6)	0.0137(18)
C2a	0.3445(9)	0.6756(6)	0.4393(6)	0.0122(17)
C3a	0.5061(10)	0.7386(7)	0.5157(5)	0.0122(16)
C4a	0.6544(9)	0.8459(6)	0.4556(6)	0.0137(18)
C5a	0.6377(10)	0.8958(6)	0.3181(6)	0.0118(17)
C6a	0.4783(10)	0.8321(6)	0.2423(6)	0.0157(18)
C7a	0.1652(10)	0.6578(6)	0.2098(6)	0.0147(18)
C8a	0.5149(11)	0.6964(7)	-0.3346(5)	0.0140(17)
C9a	0.2275(10)	0.9740(6)	-0.2545(6)	0.0132(18)
H1c4	0.7695	0.8862	0.5091	0.016397
H1c6	0.4691	0.8644	0.1468	0.018791
H1c2	0.2428	0.6005	0.4815	0.014685

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Th-btc-VI The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	0.01371(9)	0.01371(9)	0.00697(8)	-0.00738(6)	-0.00188(9)	0.00159(9)
O1h	0.011(2)	0.022(2)	0.008(2)	-0.0057(16)	-0.0010(17)	0.0013(17)
O1w	0.023(2)	0.034(3)	0.024(3)	0.000(2)	-0.006(2)	-0.010(2)
O71a	0.035(3)	0.029(3)	0.008(2)	-0.0136(19)	-0.0102(18)	0.0003(18)
O72a	0.027(2)	0.018(2)	0.014(2)	-0.0144(18)	-0.0024(18)	0.0006(17)
O81a	0.022(2)	0.019(2)	0.013(2)	-0.0115(17)	0.0036(18)	0.0021(17)
O82a	0.021(2)	0.030(3)	0.009(2)	-0.0120(19)	-0.0061(18)	0.0027(18)
O91a	0.026(2)	0.0173(19)	0.0077(18)	-0.0094(15)	-0.003(2)	0.0004(19)
O92a	0.032(3)	0.033(3)	0.014(2)	-0.023(2)	-0.008(2)	0.003(2)
C1a	0.017(3)	0.011(3)	0.013(3)	-0.003(2)	-0.003(2)	-0.001(2)
C2a	0.011(3)	0.012(3)	0.014(3)	-0.002(2)	0.003(2)	-0.002(2)
C3a	0.012(3)	0.012(3)	0.011(3)	-0.002(2)	0.004(3)	0.005(2)
C4a	0.011(3)	0.012(3)	0.017(3)	-0.005(2)	-0.003(2)	0.001(2)
C5a	0.014(3)	0.012(3)	0.011(3)	-0.004(2)	0.000(2)	-0.004(2)

C6a	0.021(3)	0.017(3)	0.009(3)	-0.009(3)	0.003(3)	0.001(2)
C7a	0.014(3)	0.018(3)	0.012(3)	-0.007(2)	-0.003(2)	0.000(2)
C8a	0.017(3)	0.015(3)	0.010(3)	-0.004(2)	0.001(3)	-0.002(2)
C9a	0.018(3)	0.009(3)	0.013(3)	-0.003(2)	-0.001(2)	-0.003(2)

Table 4 Bond Lengths for Th-btc-VI

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	Th1	3.9101(3)		O91a	C9a	1.292(7)
Th1	O1h	2.373(4)		O92a	C9a	1.251(8)
Th1	O1h	2.408(4)		C1a	C2a	1.399(8)
Th1	O1w	2.499(5)		C1a	C6a	1.388(8)
Th1	O71a	2.440(4)		C1a	C7a	1.493(9)
Th1	O72a	2.475(4)		C2a	C3a	1.384(8)
Th1	O81a	2.399(4)		C2a	H1c2	0.96
Th1	O82a	2.375(4)		C3a	C4a	1.382(8)
Th1	O91a	2.598(4)		C3a	C8a	1.493(7)
Th1	O92a	2.642(4)		C4a	C5a	1.388(8)
O71a	C7a	1.259(7)		C4a	H1c4	0.96
O72a	C7a	1.259(7)		C5a	C6a	1.375(8)
O81a	C8a	1.259(7)		C5a	C9a	1.493(8)
O82a	C8a	1.255(8)		C6a	H1c6	0.96

II.7 Th(OH)(H$_2$O)(1,2,3-btc)

Table 1 Crystal data and structure refinement for Th(OH)(H2O)(1,2,3-btc)	
Identification code	ThO(OH)(1.2.3btc)
Empirical formula	$C_9H_3O_8Th$
Formula weight	471.15
Temperature/K	298.98
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	16.387(3)
b/Å	7.7660(13)
c/Å	8.1588(15)
α/°	90
β/°	102.826(7)
γ/°	90
Volume/Å^3	1012.4(3)
Z	4
ρ_{calc}g/cm^3	3.091
μ/mm^{-1}	14.763
F(000)	844.0
Crystal size/mm^3	0.127 × 0.056 × 0.047
Radiation	MoKα (λ = 0.71073)

2Θ range for data collection/°	2.548 to 53.284
Index ranges	$-20 \leq h \leq 20$, $-9 \leq k \leq 9$, $-10 \leq l \leq 10$
Reflections collected	16218
Independent reflections	2102 [R_{int} = 0.0433, R_{sigma} = 0.0271]
Data/restraints/parameters	2102/0/163
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0225, wR_2 = 0.0550
Final R indexes [all data]	R_1 = 0.0288, wR_2 = 0.0585
Largest diff. peak/hole / e Å^{-3}	2.50/-1.23

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th(OH)(H2O)(1,2,3-btc)U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	444.7(2)	3796.3(2)	2369.4(2)	15.00(9)
O1	-173(2)	1274(4)	1077(5)	18.0(8)
O72	1431(3)	5964(4)	1728(5)	23.3(9)
O71	-1030(3)	3577(5)	2668(5)	24.8(9)
O81	1574(2)	4300(5)	4860(5)	21.7(8)
C8	1908(3)	3984(6)	6357(7)	17.6(11)
C2	2626(3)	5168(7)	7161(7)	18.9(11)
C3	3452(4)	4636(8)	7559(8)	31.8(14)
C4	4102(4)	5737(10)	8234(10)	46.6(19)
C9	3662(4)	2871(9)	7266(10)	37.6(17)
O82	1701(2)	2834(5)	7251(5)	24.4(9)
O91	3220(4)	2076(8)	6123(8)	77.1(19)
O92	4284(5)	2214(10)	8163(12)	113(3)
C1	2461(4)	6871(7)	7465(7)	20.8(12)
C6	3109(4)	8012(8)	8096(9)	36.5(16)
C5	3923(4)	7440(9)	8472(10)	46.9(19)
C7	-1582(3)	2501(7)	2852(6)	18.9(11)
O2	495(2)	3850(4)	-674(4)	17.3(8)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Th(OH)(H2O)(1,2,3-btc)The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	21.48(13)	8.62(12)	14.26(12)	-0.10(7)	2.59(8)	0.12(7)
O1	23(2)	13.3(18)	17.3(19)	-1.8(14)	2.6(16)	-4.1(15)
O72	32(2)	12.1(19)	27(2)	0.3(16)	9.5(18)	-5.1(16)
O71	25(2)	18.6(19)	28(2)	-1.7(17)	0.6(18)	2.7(17)
O81	29(2)	21.5(19)	14.9(19)	-0.2(16)	4.7(17)	0.7(17)
C8	21(3)	13(3)	17(3)	0(2)	3(2)	6(2)
C2	19(3)	18(3)	19(3)	3(2)	2(2)	0(2)
C3	25(3)	27(3)	42(4)	2(3)	4(3)	4(3)
C4	25(3)	41(4)	70(6)	-4(4)	1(4)	-4(3)
C9	19(3)	30(4)	60(5)	-11(3)	1(3)	3(3)
O82	31(2)	17.4(19)	25(2)	5.3(17)	6.2(18)	-2.4(17)

O91	79(4)	59(4)	95(5)	-11(4)	23(4)	21(4)
O92	66(4)	84(5)	168(8)	-11(5)	-20(5)	36(4)
C1	27(3)	12(2)	24(3)	2(2)	6(2)	-2(2)
C6	38(4)	24(3)	44(4)	-9(3)	4(3)	-8(3)
C5	26(4)	43(4)	65(5)	-4(4)	-6(3)	-11(3)
C7	29(3)	16(3)	11(2)	-4(2)	4(2)	1(2)
O2	24(2)	14.8(19)	12.5(18)	-2.2(14)	3.3(15)	1.4(15)

Table 4 Bond Lengths for Th(OH)(H2O)(1,2,3-btc)

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	Th1[1]	4.1696(6)		C8	O82	1.247(6)
Th1	Th1[2]	4.1696(6)		C2	C3	1.384(8)
Th1	O1	2.345(3)		C2	C1	1.383(7)
Th1	O1[1]	2.400(3)		C3	C4	1.382(9)
Th1	O72	2.469(4)		C3	C9	1.446(9)
Th1	O71	2.488(4)		C4	C5	1.378(10)
Th1	O81	2.457(4)		C9	O91	1.215(8)
Th1	O82[3]	2.437(4)		C9	O92	1.227(9)
Th1	O2	2.503(4)		O82	Th1[5]	2.436(4)
Th1	O2[4]	2.585(3)		C1	C6	1.391(8)
Th1	O2[5]	2.592(3)		C1	C7[6]	1.488(8)
O1	Th1[2]	2.400(3)		C6	C5	1.375(9)
O72	C7[1]	1.251(6)		C7	O72[2]	1.251(6)
O71	C7	1.265(6)		C7	C1[6]	1.488(8)
O81	C8	1.247(6)		O2	Th1[4]	2.585(3)
C8	C2	1.521(7)		O2	Th1[3]	2.592(3)

[1]-X,1/2+Y,1/2-Z; [2]-X,-1/2+Y,1/2-Z; [3]+X,1/2-Y,-1/2+Z; [4]-X,1-Y,-Z; [5]+X,1/2-Y,1/2+Z; [6]-X,1-Y,1-Z

II.8 $U_2O_2(bdc)_2(H_2O)_2;(H_2O)$

Table 1 Crystal data and structure refinement for U2O2(bdc)2(H2O)2;(H2O).

Identification code	U2O2(bdc)2(H2O)2;(H2O)
Empirical formula	$C_{16}H_{14}O_{13}U_2$
Formula weight	890.33
Temperature/K	299.82
Crystal system	triclinic
Space group	P-1
a/Å	7.8178(7)
b/Å	9.5870(9)
c/Å	13.2310(13)
α/°	77.492(6)
β/°	86.775(5)
γ/°	83.487(5)
Volume/Å^3	961.36(16)

Z	2
ρ_{calc}g/cm^3	3.076
μ/mm^{-1}	16.896
F(000)	796.0
Crystal size/mm^3	0.138 × 0.06 × 0.056
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.154 to 52.78
Index ranges	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	24286
Independent reflections	3929 [R_{int} = 0.0581, R_{sigma} = 0.0448]
Data/restraints/parameters	3929/0/285
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0255, wR_2 = 0.0498
Final R indexes [all data]	R_1 = 0.0397, wR_2 = 0.0546
Largest diff. peak/hole / e Å^{-3}	1.23/-1.04

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U2O2(bdc)2(H2O)2;(H2O). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U001	6432.7(3)	8290.2(2)	5212.5(2)	11.07(7)
U002	1357.4(3)	8820.4(3)	4239.1(2)	12.28(8)
O2H	3798(5)	9220(5)	4782(3)	13.1(10)
O71A	5890(6)	8383(5)	6947(4)	22.9(11)
O2W	8306(6)	6163(5)	6379(4)	25.3(12)
O81B	8173(6)	3196(5)	4300(4)	18.4(11)
O72A	7005(6)	10204(5)	7373(4)	24.9(12)
O81A	3168(6)	10698(5)	6609(3)	18.5(11)
O72B	9800(7)	7069(5)	3707(5)	41.0(16)
O82B	5341(6)	3668(5)	4060(4)	27.0(13)
O82A	630(6)	9895(5)	7134(4)	26.4(12)
C7A	5958(9)	9303(8)	7514(5)	18.3(16)
C8A	2184(9)	10037(7)	7281(5)	17.7(15)
O1W	3314(7)	6747(5)	3616(4)	36.8(14)
C2B	7293(9)	4744(7)	2752(5)	17.9(16)
O1H	9010(5)	8969(4)	5311(3)	13.5(10)
C1A	4706(9)	9117(7)	8423(5)	16.8(15)
O3W	9151(10)	7178(10)	8151(8)	88(3)
O71B	7225(8)	6385(5)	4289(4)	35.1(14)
C1B	8251(8)	5900(7)	2689(5)	15.1(15)
C3A	1849(9)	9136(8)	9185(5)	23.5(17)
C4A	2511(10)	8560(8)	10149(6)	32(2)
C6A	5360(10)	8538(8)	9387(5)	23.6(17)
C7B	8456(9)	6475(7)	3618(6)	22.5(17)
C8B	6874(9)	3808(7)	3791(5)	18.7(16)
C5A	4264(10)	8238(9)	10248(6)	31(2)
C2A	2921(9)	9405(7)	8313(5)	15.9(15)
C5B	8506(11)	6157(9)	855(6)	42(2)
C4B	7451(12)	5076(9)	913(6)	43(2)

C6B	8859(10)	6584(8)	1732(6)	29.6(19)
C3B	6862(11)	4373(8)	1863(6)	31(2)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U2O2(bdc)2(H2O)2;(H2O). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U001	6.15(13)	9.43(14)	17.51(15)	-2.64(11)	0.57(10)	-1.23(9)
U002	6.45(13)	11.37(14)	19.57(16)	-4.22(11)	0.15(10)	-1.76(10)
O2H	6(2)	12(2)	21(3)	-4(2)	1.1(18)	-1.1(18)
O71A	31(3)	19(3)	18(3)	-6(2)	4(2)	4(2)
O2W	20(3)	27(3)	26(3)	1(2)	-3(2)	-1(2)
O81B	8(2)	13(3)	30(3)	3(2)	2(2)	0.1(19)
O72A	17(3)	40(3)	19(3)	-5(2)	2(2)	-13(2)
O81A	15(3)	22(3)	14(3)	4(2)	3(2)	0(2)
O72B	30(3)	25(3)	74(4)	-19(3)	-26(3)	-4(3)
O82B	14(3)	13(3)	47(4)	9(2)	-1(2)	-1(2)
O82A	12(3)	35(3)	28(3)	5(2)	-6(2)	-6(2)
C7A	14(4)	26(4)	11(4)	1(3)	-1(3)	9(3)
C8A	18(4)	16(4)	19(4)	-7(3)	3(3)	5(3)
O1W	30(3)	29(3)	53(4)	-19(3)	5(3)	8(3)
C2B	16(4)	15(4)	24(4)	-8(3)	1(3)	2(3)
O1H	7(2)	10(2)	24(3)	-5(2)	4.8(19)	-3.8(18)
C1A	16(4)	16(4)	19(4)	-6(3)	6(3)	-4(3)
O3W	62(6)	92(7)	100(7)	-11(6)	-17(5)	19(5)
O71B	64(4)	21(3)	20(3)	-8(2)	14(3)	-6(3)
C1B	12(4)	14(4)	20(4)	-7(3)	5(3)	-3(3)
C3A	17(4)	27(4)	24(4)	-3(3)	3(3)	0(3)
C4A	30(5)	40(5)	20(4)	0(4)	14(3)	-2(4)
C6A	20(4)	30(5)	19(4)	2(3)	-3(3)	-5(3)
C7B	20(4)	9(4)	36(5)	-1(3)	-8(3)	3(3)
C8B	18(4)	15(4)	24(4)	-3(3)	-1(3)	-5(3)
C5A	33(5)	36(5)	23(5)	0(4)	-6(4)	-4(4)
C2A	18(4)	19(4)	11(4)	1(3)	-2(3)	-5(3)
C5B	53(6)	46(6)	15(5)	9(4)	3(4)	13(5)
C4B	68(7)	39(6)	21(5)	-9(4)	-16(4)	6(5)
C6B	25(4)	26(5)	36(5)	0(4)	9(4)	-10(3)
C3B	52(6)	16(4)	27(5)	-6(4)	-16(4)	-5(4)

Table 4 Bond Lengths for U2O2(bdc)2(H2O)2;(H2O).

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U001	$U001^1$	3.7094(6)		O81A	$U001^1$	2.411(4)
U001	$U002^1$	3.6444(4)		O81A	C8A	1.255(8)
U001	$U002^2$	4.0426(5)		O72B	$U002^2$	2.423(5)
U001	O2H	2.204(4)		O72B	C7B	1.273(8)
U001	$O2H^1$	2.375(4)		O82B	$U001^3$	2.456(5)

U001	O71A	2.329(5)		O82B	C8B	1.245(8)
U001	O2W	2.627(4)		O82A	U002[5]	2.479(4)
U001	O81A[1]	2.411(4)		O82A	C8A	1.268(8)
U001	O82B[3]	2.456(5)		C7A	C1A	1.500(9)
U001	O1H	2.205(4)		C8A	C2A	1.488(9)
U001	O71B	2.417(5)		C2B	C1B	1.393(9)
U002	U001[4]	4.0426(5)		C2B	C8B	1.511(9)
U002	U001[1]	3.6445(4)		C2B	C3B	1.369(9)
U002	U002[5]	3.7519(6)		O1H	U002[2]	2.266(4)
U002	O2H	2.178(4)		O1H	U002[1]	2.306(4)
U002	O81B[3]	2.431(4)		C1A	C6A	1.379(9)
U002	O72A[1]	2.483(5)		C1A	C2A	1.401(9)
U002	O72B[4]	2.423(5)		O71B	C7B	1.269(9)
U002	O82A[5]	2.479(4)		C1B	C7B	1.475(10)
U002	O1W	2.616(5)		C1B	C6B	1.379(10)
U002	O1H[1]	2.306(4)		C3A	C4A	1.380(10)
U002	O1H[4]	2.266(4)		C3A	C2A	1.383(9)
O2H	U001[1]	2.375(4)		C4A	C5A	1.378(11)
O71A	C7A	1.283(8)		C6A	C5A	1.384(10)
O81B	U002[3]	2.431(4)		C5B	C4B	1.383(12)
O81B	C8B	1.265(8)		C5B	C6B	1.363(11)
O72A	U002[1]	2.483(5)		C4B	C3B	1.373(11)
O72A	C7A	1.234(8)				

[1]1-X,2-Y,1-Z; [2]1+X,+Y,+Z; [3]1-X,1-Y,1-Z; [4]-1+X,+Y,+Z; [5]-X,2-Y,1-Z

II.9 $Np_2O_2(bdc)_2(H_2O)_2;(H_2O)$

Table 1 Crystal data and structure refinement for Np2O2(bdc)2(H2O)2;(H2O).	
Identification code	Np2O2(bdc)2(H2O)2;(H2O)
Empirical formula	$C_{16}H_{12}Np_2O_{13}$
Formula weight	886.26
Temperature/K	100
Crystal system	triclinic
Space group	P-1
a/Å	7.8178(7)
b/Å	9.5870(9)
c/Å	13.2310(13)
α/°	77.492(6)
β/°	86.775(5)
γ/°	83.487(5)
Volume/Å^3	961.36(16)
Z	2
ρ_{calc}g/cm^3	3.062
μ/mm^{-1}	10.821

F(000)	796.0
Crystal size/mm^3	0.132 × 0.06 × 0.055
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.822 to 52.572
Index ranges	-9 ≤ h ≤ 9, -11 ≤ k ≤ 11, -16 ≤ l ≤ 16
Reflections collected	61364
Independent reflections	3862 [R_{int} = 0.0587, R_{sigma} = 0.0264]
Data/restraints/parameters	3862/0/257
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0217, wR_2 = 0.0393
Final R indexes [all data]	R_1 = 0.0344, wR_2 = 0.0418
Largest diff. peak/hole / e Å^{-3}	1.02/-0.98

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np2O2(bdc)2(H2O)2;(H2O). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	6428.1(2)	8292.0(2)	5206.8(2)	4.12(6)
Np2	1352.2(2)	8833.3(2)	4231.3(2)	4.56(6)
O2	3809(4)	9239(4)	4763(3)	7.1(7)
O71A	5846(4)	8352(4)	6950(3)	10.4(8)
O2W	8282(4)	6174(4)	6391(3)	10.8(8)
O81B	8182(4)	3173(4)	4302(3)	9.3(7)
O72A	7050(4)	10166(4)	7386(3)	11.0(8)
O72B	9828(5)	7095(4)	3635(3)	20.5(9)
O82B	5318(4)	3672(4)	4118(3)	11.1(8)
O82A	638(4)	9841(4)	7134(3)	10.5(8)
O81A	3152(4)	10713(4)	6607(3)	7.1(7)
O1W	3290(5)	6737(4)	3625(3)	15.4(8)
O1	9012(4)	8972(3)	5299(3)	6.6(7)
C1A	4720(6)	9121(5)	8443(4)	7.3(10)
O3W	9184(5)	7193(4)	8144(3)	25.5(10)
O71B	7310(5)	6380(4)	4296(3)	15.4(8)
C1B	8228(6)	5893(5)	2668(4)	6.9(10)
C3A	1835(6)	9135(5)	9222(4)	10.6(11)
C4A	2518(7)	8565(6)	10196(4)	13.1(12)
C6A	5379(6)	8532(5)	9425(4)	10.1(11)
C8B	6861(6)	3809(5)	3818(4)	8.4(11)
C5A	4282(7)	8240(5)	10292(4)	12.6(11)
C2A	2909(6)	9399(5)	8338(4)	6.5(10)
C5B	8424(7)	6102(6)	805(4)	20.9(14)
C4B	7348(8)	5004(6)	894(4)	21.9(14)
C6B	8836(7)	6560(6)	1689(4)	14.7(12)
C3B	6752(7)	4321(6)	1875(4)	15.7(12)
C2B	7227(6)	4735(5)	2761(4)	7.7(10)
C7B	8485(6)	6494(5)	3602(4)	7.3(10)
C8A	2187(6)	10020(5)	7280(4)	8.8(11)
C7A	5964(6)	9260(5)	7518(4)	7.4(10)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Np2O2(bdc)2(H2O)2;(H2O). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	1.59(10)	2.99(10)	7.48(11)	-0.23(8)	0.15(8)	-0.74(8)
Np2	1.47(10)	3.68(11)	8.49(11)	-0.77(8)	-0.06(8)	-1.15(8)
O2	1.7(16)	6.8(17)	12.3(19)	-0.3(14)	-0.3(14)	-1.9(13)
O71A	11.9(18)	8.0(18)	9.9(19)	0.4(15)	0.3(15)	-0.5(15)
O2W	8.6(18)	10.4(19)	13(2)	-2.0(15)	1.1(15)	0.0(15)
O81B	4.8(17)	8.2(18)	13.1(19)	1.3(15)	1.1(14)	-0.2(14)
O72A	5.0(17)	15(2)	12.2(19)	-0.2(16)	0.5(14)	-3.2(15)
O72B	11.2(19)	12(2)	41(3)	-9.1(19)	-11.3(18)	0.4(16)
O82B	4.0(17)	7.9(18)	20(2)	1.3(15)	0.3(15)	-1.6(14)
O82A	2.8(17)	15(2)	12.3(19)	1.1(16)	-1.7(14)	-3.4(14)
O1W	12.6(19)	13(2)	21(2)	-6.4(17)	-1.2(16)	2.3(16)
O1	4.3(16)	4.4(17)	10.7(18)	-0.3(14)	-0.9(14)	-0.5(13)
C1A	8(2)	3(2)	11(3)	-2(2)	1(2)	-0.6(19)
O3W	23(2)	29(2)	24(2)	-2.3(19)	-3.0(18)	-2.7(19)
O71B	31(2)	6.0(18)	9.2(19)	-3.0(15)	4.5(17)	-3.0(16)
C3A	6(2)	9(3)	17(3)	-4(2)	2(2)	0(2)
C4A	13(3)	13(3)	12(3)	-2(2)	6(2)	-4(2)
C6A	7(2)	15(3)	8(3)	0(2)	-1(2)	-4(2)
C8B	8(3)	3(2)	13(3)	0(2)	-2(2)	1(2)
C5A	14(3)	11(3)	12(3)	-1(2)	-5(2)	-2(2)
C2A	6(2)	4(2)	9(3)	2(2)	-1(2)	-3.4(19)
C5B	24(3)	19(3)	14(3)	2(2)	5(2)	12(3)
C4B	29(3)	24(3)	13(3)	-9(3)	-6(3)	10(3)
C6B	14(3)	8(3)	18(3)	5(2)	5(2)	0(2)
C3B	17(3)	9(3)	22(3)	-3(2)	-5(2)	-3(2)
C8A	12(3)	3(2)	10(3)	-1(2)	1(2)	1(2)

Table 4 Bond Lengths for Np2O2(bdc)2(H2O)2;(H2O).

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	$Np1^1$	3.7031(5)		O72B	$Np2^2$	2.438(4)
Np1	$Np2^2$	4.0445(4)		O72B	C7B	1.261(6)
Np1	$Np2^1$	3.6438(4)		O82B	$Np1^3$	2.434(3)
Np1	$O2^1$	2.362(3)		O82B	C8B	1.260(6)
Np1	O2	2.201(3)		O82A	$Np2^5$	2.484(3)
Np1	O71A	2.338(3)		O82A	C8A	1.273(6)
Np1	O2W	2.625(3)		O81A	$Np1^1$	2.402(3)
Np1	$O82B^3$	2.434(3)		O81A	C8A	1.259(6)
Np1	$O81A^1$	2.402(3)		O1	$Np2^2$	2.258(3)
Np1	O1	2.210(3)		O1	$Np2^1$	2.303(3)
Np1	O71B	2.422(3)		C1A	C6A	1.401(7)
Np2	$Np1^4$	4.0445(4)		C1A	C2A	1.419(7)
Np2	$Np1^1$	3.6438(4)		C1A	C7A	1.513(7)

Np2	Np2[5]	3.7452(5)		O71B	C7B	1.258(6)
Np2	O2	2.185(3)		C1B	C6B	1.398(7)
Np2	O81B[3]	2.429(3)		C1B	C2B	1.410(7)
Np2	O72A[1]	2.479(3)		C1B	C7B	1.504(7)
Np2	O72B[4]	2.438(4)		C3A	C4A	1.397(7)
Np2	O82A[5]	2.484(3)		C3A	C2A	1.394(7)
Np2	O1W	2.617(3)		C4A	C5A	1.385(7)
Np2	O1[4]	2.258(3)		C6A	C5A	1.391(7)
Np2	O1[1]	2.303(3)		C8B	C2B	1.516(7)
O2	Np1[1]	2.362(3)		C2A	C8A	1.512(7)
O71A	C7A	1.280(6)		C5B	C4B	1.402(8)
O81B	Np2[3]	2.429(3)		C5B	C6B	1.401(8)
O81B	C8B	1.270(6)		C4B	C3B	1.401(8)
O72A	Np2[1]	2.479(3)		C3B	C2B	1.398(7)
O72A	C7A	1.261(6)				

[1]1-X,2-Y,1-Z; [2]1+X,+Y,+Z; [3]1-X,1-Y,1-Z; [4]-1+X,+Y,+Z; [5]-X,2-Y,1-Z

II.10 $U_2(OH)_2(mel)(H_2O)_2$

Table 1 Crystal data and structure refinement for U2(OH)2(mel)(H2O)2.	
Identification code	U2(OH)2(mel)(H2O)2
Empirical formula	$C_6H_2O_8U$
Formula weight	440.11
Temperature/K	299.48
Crystal system	orthorhombic
Space group	Fdd2
a/Å	13.903(3)
b/Å	19.813(5)
c/Å	11.393(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3138.4(14)
Z	16
ρ_{calc}g/cm^3	3.726
μ/mm^{-1}	20.714
F(000)	3104.0
Crystal size/mm^3	0.091 × 0.073 × 0.057
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.06 to 52.908
Index ranges	-17 ≤ h ≤ 17, -24 ≤ k ≤ 23, -14 ≤ l ≤ 14
Reflections collected	13003
Independent reflections	1589 [R_{int} = 0.0907, R_{sigma} = 0.0752]
Data/restraints/parameters	1589/1/131

Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0477, wR_2 = 0.0995
Final R indexes [all data]	R_1 = 0.0707, wR_2 = 0.1078
Largest diff. peak/hole / e $Å^{-3}$	2.86/-1.72
Flack parameter	0.507(17)

Table 2 Fractional Atomic Coordinates ($\times10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2\times10^3$) for U2(OH)2(mel)(H2O)2. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U001	6181.9(5)	2727.8(6)	5056(3)	22.8(3)
O1OH	7218(9)	1852(10)	5047(19)	26(4)
O62	3976(13)	3570(13)	3132(17)	33(6)
C6	4104(18)	3080(18)	3740(20)	22(7)
O1W	5287(14)	1737(12)	5900(20)	36(5)
O61	4884(12)	2743(13)	3821(16)	33(6)
O81	6737(14)	2711(11)	3084(17)	24(6)
O51	6743(13)	2686(11)	7036(16)	23(6)
C3	3270(20)	2801(16)	5670(20)	19(7)
C2	3258(19)	2776(15)	4430(20)	15(6)
C5	2500	2500	2520(50)	23(8)
C8	7500	2500	2580(50)	22(8)
O71	6096(11)	3882(11)	4629(14)	24(5)
C1	2500	2500	3870(30)	18(9)
C4	2500	2500	6300(40)	30(12)
O72	7347(11)	4294(12)	3652(16)	27(5)
C7	6480(20)	4280(20)	3840(30)	28(8)

Table 3 Anisotropic Displacement Parameters ($Å^2\times10^3$) for U2(OH)2(mel)(H2O)2. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U001	18.1(4)	36.0(6)	14.3(4)	0.8(4)	0.1(4)	2.6(5)
O1OH	20(7)	40(13)	18(8)	-5(10)	1(9)	-1(8)
O62	27(10)	51(18)	20(10)	5(11)	7(8)	-3(10)
C6	17(12)	40(20)	8(12)	-3(13)	0(10)	-7(13)
O1W	35(10)	27(15)	45(12)	-2(11)	-14(9)	1(10)
O61	10(8)	70(20)	18(9)	-6(11)	-1(7)	-14(11)
O81	19(10)	35(18)	17(10)	-1(8)	-4(8)	-2(9)
O51	18(10)	45(19)	6(9)	6(8)	-4(8)	6(9)
C3	23(12)	26(19)	8(12)	-12(11)	-4(9)	3(12)
C5	20(16)	40(30)	7(15)	0	0	0(17)
C8	15(15)	30(20)	17(16)	0	0	-5(16)
O71	12(7)	44(15)	17(9)	10(8)	3(6)	11(9)
C4	40(20)	40(30)	12(18)	0	0	0(20)
O72	7(8)	48(17)	27(10)	-1(10)	4(7)	4(9)
C7	23(13)	40(20)	18(14)	-18(14)	0(11)	3(14)

Table 4 Bond Lengths for U2(OH)2(mel)(H2O)2.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
U001	U001[1]	3.7746(17)		C3	C4	1.42(4)
U001	O1OH	2.255(17)		C3	C7[2]	1.51(4)
U001	O1OH[1]	2.376(14)		C2	C1	1.35(3)
U001	O1W	2.52(2)		C5	O51[4]	1.24(3)
U001	O61	2.288(18)		C5	O51[5]	1.24(3)
U001	O81	2.38(2)		C5	C1	1.54(7)
U001	O51	2.388(19)		C8	O81[1]	1.28(3)
U001	O71	2.34(2)		C8	C4[6]	1.46(7)
U001	O72[2]	2.430(18)		O71	C7	1.31(4)
O1OH	U001[1]	2.376(14)		C1	C2[7]	1.35(3)
O62	C6	1.20(4)		C4	C3[7]	1.42(4)
C6	O61	1.28(4)		C4	C8[8]	1.46(7)
C6	C2	1.54(4)		O72	U001[9]	2.430(18)
O81	C8	1.28(3)		O72	C7	1.22(3)
O51	C5[3]	1.24(3)		C7	C3[9]	1.51(4)
C3	C2	1.41(3)				

[1]3/2-X,1/2-Y,+Z; [2]-1/4+X,3/4-Y,1/4+Z; [3]1/2+X,+Y,1/2+Z; [4]-1/2+X,+Y,-1/2+Z; [5]1-X,1/2-Y,-1/2+Z; [6]1/2+X,+Y,-1/2+Z; [7]1/2-X,1/2-Y,+Z; [8]-1/2+X,+Y,1/2+Z; [9]1/4+X,3/4-Y,-1/4+Z

II.11 [(NpO$_2$)$_{10}$(H$_2$O)$_{14}$(Hmel)$_2$]·12H$_2$O

Table 1 Crystal data and structure refinement for [(NpO2)10(H2O)14(Hmel)2]·12H2O.	
Identification code	[(NpO2)10(H2O)14(Hmel)2]·12H2O
Empirical formula	$Np_{20}C_{48}O_{140}H$
Formula weight	7556.48
Temperature/K	293(2)
Crystal system	monoclinic
Space group	Pn
a/Å	12.965
b/Å	12.980
c/Å	20.104
α/°	90
β/°	95.17
γ/°	90
Volume/Å^3	3369.3
Z	1
ρ_{calc}g/cm^3	3.724
μ/mm^{-1}	15.407
F(000)	3268.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71069)

2Θ range for data collection/°	4.45 to 53.334
Index ranges	$-16 \leq h \leq 16$, $-16 \leq k \leq 16$, $-25 \leq l \leq 25$
Reflections collected	152644
Independent reflections	13813 [R_{int} = 0.1276, R_{sigma} = 0.0493]
Data/restraints/parameters	13813/2/467
Goodness-of-fit on F^2	2.972
Final R indexes [I>=2σ (I)]	R_1 = 0.1454, wR_2 = 0.3348
Final R indexes [all data]	R_1 = 0.1484, wR_2 = 0.3367
Largest diff. peak/hole / e $Å^{-3}$	10.79/-14.26
Flack parameter	0.116(11)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for [(NpO2)10(H2O)14(Hmel)2]·12H2O. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	3990(2)	8754(3)	3685.2(18)	10.7(8)
Np2	2798(2)	5881(2)	3042.3(17)	9.7(8)
Np3	1983(3)	12852(2)	3383(2)	10.0(7)
Np4	105(2)	6967(3)	3717.9(18)	10.3(8)
Np5	989(2)	9787(2)	3020.9(17)	10.6(8)
Np6	6953(3)	7820(3)	3354(2)	11.4(7)
Np7	-1975(2)	10913(3)	3419.2(17)	10.6(8)
Np8	5085(2)	11764(2)	3326.3(17)	11.2(8)
Np9	8921(2)	3943(3)	3348.2(17)	11.5(8)
Np10	5854(3)	4755(3)	3387.6(19)	13.6(8)
O1	600(50)	13260(50)	3470(30)	3(13)
O2	9460(50)	5170(50)	3630(30)	24(13)
O3	4610(50)	10570(50)	3610(30)	13(14)
O4	4540(50)	5240(50)	3100(40)	8(14)
O5	7180(50)	4320(50)	3660(30)	22(13)
O6	4980(50)	12190(50)	4610(30)	14(13)
O7	7140(70)	7620(70)	4550(50)	40(20)
O8	7340(50)	9200(40)	3400(30)	19(12)
O9	4740(40)	13420(40)	7530(30)	19(11)
O10	1650(50)	12850(40)	2130(40)	18(13)
O11	-2540(50)	10690(50)	2130(40)	17(15)
O12	-4190(50)	10060(50)	-810(30)	10(12)
O13	9040(50)	3580(50)	4580(30)	24(12)
O14	3360(50)	12460(50)	3370(40)	19(14)
O15	3340(50)	15430(50)	4220(30)	17(13)
O16	3150(50)	15170(40)	7350(30)	12(12)
O17	2130(50)	9170(50)	2170(30)	22(13)
O18	3400(50)	7550(50)	4590(40)	16(15)
O19	-4370(50)	11710(50)	-440(30)	14(13)
O20	6380(50)	13560(50)	7190(30)	22(13)
O21	1510(50)	11130(50)	3030(30)	6(12)
O22	210(50)	10100(50)	1860(30)	18(13)
O23	1790(50)	11890(50)	4430(30)	14(13)
O24	1460(50)	6440(50)	3690(30)	12(13)

O25	-3970(50)	10740(50)	2640(30)	22(13)
O26	-6480(50)	9970(50)	-470(30)	17(12)
O27	2640(50)	9340(50)	3580(30)	11(12)
O28	4160(50)	11710(50)	2180(40)	31(15)
O29	5260(50)	8230(40)	3780(30)	12(12)
O30	7800(50)	7420(50)	2290(30)	26(13)
O31	4980(50)	13690(50)	4090(40)	7(14)
O32	4690(50)	15820(50)	7260(40)	10(14)
O33	-770(40)	10450(40)	3140(30)	8(12)
O34	3340(50)	5760(50)	1880(30)	15(13)
O35	-1580(50)	9060(50)	1540(40)	15(14)
O36	2260(50)	4590(50)	2960(30)	8(13)
O37	6560(50)	6500(50)	3280(30)	12(13)
O38	-4160(50)	8360(50)	2440(40)	22(14)
O39	-5810(40)	8480(40)	-590(30)	13(12)
O40	3480(50)	11190(50)	5170(40)	33(15)
O41	-3530(50)	12330(50)	1140(40)	30(14)
O42	6440(90)	10000(80)	5230(60)	60(30)
O43	2650(40)	13850(40)	4330(30)	8(12)
C1	3890(60)	15230(60)	7000(40)	17(16)
O44	-400(70)	12070(70)	1520(60)	40(20)
O45	10960(50)	3500(50)	5190(40)	30(14)
O46	6770(50)	13100(50)	5590(40)	26(14)
O47	-3090(50)	11430(50)	3840(40)	23(14)
O48	2330(70)	11130(70)	1460(50)	33(19)
O49	-2410(50)	11390(50)	570(40)	27(14)
C2	-4840(70)	9380(70)	1560(50)	19(17)
O50	-5950(50)	7530(50)	1380(30)	15(13)
O51	5610(50)	12950(50)	2930(40)	22(13)
O52	1880(50)	15520(50)	5350(40)	40(15)
O53	2840(50)	16400(50)	6150(40)	27(15)
O54	8080(60)	5340(60)	5020(40)	37(17)
O55	6030(50)	11920(50)	6180(40)	26(15)
O56	4280(90)	13670(90)	1620(70)	90(30)
C3	-4320(70)	10700(60)	-360(50)	5(17)
O57	8450(50)	2690(50)	3070(30)	24(12)
O58	6040(50)	6590(50)	1560(30)	15(13)
C4	-4970(70)	8880(70)	2220(50)	13(17)
C5	-3960(70)	10600(70)	900(50)	21(17)
C6	5140(60)	13420(60)	5880(50)	10(16)
C7	-5370(60)	9080(60)	980(40)	8(16)
C8	-3200(60)	11470(60)	860(50)	15(17)
O59	5410(100)	7160(90)	5220(80)	90(30)
C9	-5260(60)	9520(60)	330(40)	5(16)
O60	-1270(50)	7410(50)	3730(40)	11(13)
C10	4920(70)	13170(70)	4640(50)	20(18)
O61	-5750(50)	9060(40)	2520(30)	15(12)
O62	-6930(50)	8260(50)	560(40)	17(14)

C11	2620(70)	15640(70)	5760(50)	26(18)
C12	5450(70)	13660(70)	7170(50)	21(19)
C13	6030(70)	12680(60)	5900(50)	17(17)
C14	-3510(60)	10590(60)	2110(40)	8(14)
C15	-6190(70)	8150(60)	970(50)	14(16)
O63	6120(50)	4770(50)	2210(40)	21(14)
O64	4430(40)	9370(50)	4810(30)	8(12)
C16	4640(70)	13640(70)	5240(50)	12(17)
O65	30(50)	6320(50)	4870(30)	15(13)
O66	5950(80)	5630(80)	4500(60)	70(30)
C17	4880(60)	13960(60)	6450(40)	9(15)
O67	530(50)	8430(50)	3050(30)	11(13)
C18	4040(60)	14650(60)	6380(40)	15(15)
C19	-5910(70)	9270(70)	-260(50)	19(17)
C20	3150(70)	14630(70)	4520(50)	13(19)
O68	1880(110)	14490(100)	1210(80)	30(40)
C21	-4440(80)	10280(70)	320(50)	20(20)
O69	3360(50)	7180(50)	3120(40)	9(14)
O70	8880(100)	7670(100)	5550(80)	70(40)
C22	3780(60)	14390(60)	5210(40)	6(16)
C23	-4100(70)	10170(60)	1510(50)	15(17)
C24	3560(60)	14930(60)	5790(40)	14(16)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for [(NpO2)10(H2O)14(Hmel)2]·12H2O. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	10.1(16)	10.4(15)	11.7(16)	-0.5(13)	1.1(13)	-0.1(12)
Np2	9.7(16)	8.9(16)	10.3(16)	-0.1(12)	-0.5(13)	0.5(12)
Np3	9.1(15)	9.5(14)	11.3(16)	-0.6(12)	-0.2(12)	-0.3(12)
Np4	13.0(16)	8.0(14)	10.2(17)	0.3(13)	2.1(13)	-0.9(12)
Np5	11.4(16)	9.9(16)	10.6(16)	-0.7(12)	1.3(13)	0.3(12)
Np6	10.9(15)	11.0(15)	12.4(16)	0.7(12)	1.7(12)	-0.1(12)
Np7	11.3(16)	9.3(15)	10.9(17)	-1.4(12)	-1.1(13)	0.3(12)
Np8	12.3(16)	10.8(15)	10.8(17)	-1.2(13)	2.1(13)	-0.3(12)
Np9	11.6(16)	8.8(15)	14.1(17)	0.8(13)	1.2(13)	0.2(12)
Np10	12.6(17)	13.3(17)	14.8(18)	0.5(13)	1.3(14)	-0.1(13)

Table 4 Bond Lengths for [(NpO2)10(H2O)14(Hmel)2]·12H2O.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	O3	2.50(6)		Np10	$O51^2$	2.53(6)
Np1	O18	2.57(7)		Np10	O63	2.42(7)
Np1	O27	1.91(6)		Np10	O66	2.51(12)
Np1	O29	1.78(6)		O1	$Np9^7$	2.34(6)
Np1	$O61^1$	2.42(6)		O2	$Np4^1$	2.48(6)
Np1	O64	2.42(6)		O6	C10	1.28(11)

Np1	O69	2.45(7)		O8	Np7[1]	2.39(6)
Np2	O4	2.40(7)		O9	Np4[6]	2.44(6)
Np2	O15[2]	2.48(7)		O9	C12	1.25(11)
Np2	O20[3]	2.50(6)		O11	C14	1.26(10)
Np2	O24	2.37(6)		O12	Np5[3]	2.38(7)
Np2	O34	2.50(7)		O12	C3	1.25(11)
Np2	O36	1.82(6)		O15	Np2[4]	2.48(7)
Np2	O69	1.84(6)		O15	C20	1.24(11)
Np3	O1	1.89(6)		O16	Np9[10]	2.45(6)
Np3	O10	2.52(7)		O16	C1	1.24(10)
Np3	O14	1.86(7)		O19	Np4[3]	2.47(6)
Np3	O21	2.41(6)		O19	C3	1.31(10)
Np3	O23	2.48(7)		O20	Np2[6]	2.50(6)
Np3	O36[4]	2.45(6)		O20	C12	1.21(11)
Np3	O43	2.40(6)		O25	Np8[5]	2.33(6)
Np4	O2[5]	2.48(6)		O25	C14	1.28(10)
Np4	O9[3]	2.44(6)		O26	Np7[3]	2.53(7)
Np4	O19[6]	2.47(6)		O26	C19	1.22(11)
Np4	O24	1.89(6)		O31	Np10[4]	2.34(7)
Np4	O60	1.88(6)		O31	C10	1.31(12)
Np4	O65	2.47(7)		O32	Np9[10]	2.49(7)
Np4	O67	2.42(6)		O32	C1	1.36(11)
Np5	O12[6]	2.38(7)		O36	Np3[2]	2.45(6)
Np5	O17	2.49(6)		O38	Np6[5]	2.35(7)
Np5	O21	1.86(6)		O38	C4	1.28(11)
Np5	O22	2.50(7)		O39	Np7[3]	2.51(6)
Np5	O27	2.39(6)		O39	C19	1.23(11)
Np5	O33	2.47(6)		O41	C8	1.33(11)
Np5	O67	1.87(6)		O43	C20	1.24(11)
Np6	O7	2.42(11)		C1	Np9[10]	2.91(9)
Np6	O8	1.86(6)		C1	C18	1.48(11)
Np6	O29	2.48(6)		O46	C13	1.31(11)
Np6	O30	2.55(7)		O47	Np8[5]	2.53(7)
Np6	O37	1.79(6)		O49	C8	1.22(11)
Np6	O38[1]	2.35(7)		C2	C4	1.51(13)
Np6	O60[1]	2.42(7)		C2	C7	1.35(13)
Np7	Np8[5]	3.957(5)		C2	C23	1.41(12)
Np7	O8[5]	2.39(6)		O50	C15	1.17(11)
Np7	O11	2.64(7)		O51	Np10[4]	2.53(6)
Np7	O25	2.90(6)		O52	C11	1.22(12)
Np7	O26[6]	2.53(7)		O53	C11	1.27(11)
Np7	O33	1.81(6)		O55	C13	1.13(11)
Np7	O39[6]	2.51(6)		C3	C21	1.51(13)
Np7	O47	1.87(7)		O57	Np7[8]	2.48(6)
Np7	O57[7]	2.48(6)		C4	O61	1.25(11)
Np7	C19[6]	2.88(9)		C5	C8	1.51(12)
Np8	Np7[1]	3.957(5)		C5	C21	1.33(14)
Np8	Np10[4]	4.007(5)		C5	C23	1.38(13)

Np8	O3	1.78(7)		C6	C13	1.50(11)
Np8	O6	2.66(7)		C6	C16	1.43(13)
Np8	O14	2.41(7)		C6	C17	1.40(12)
Np8	O25[1]	2.33(6)		C7	C9	1.44(12)
Np8	O28	2.51(7)		C7	C15	1.61(11)
Np8	O47[1]	2.53(7)		C9	C19	1.43(12)
Np8	O51	1.89(6)		C9	C21	1.45(13)
Np9	O1[8]	2.34(6)		O60	Np6[5]	2.42(7)
Np9	O2	1.81(6)		C10	C16	1.43(13)
Np9	O5	2.45(6)		O61	Np1[5]	2.42(6)
Np9	O13	2.52(6)		O62	C15	1.23(12)
Np9	O16[9]	2.45(6)		C11	C24	1.52(12)
Np9	O32[9]	2.49(7)		C12	C17	1.62(13)
Np9	C1[9]	2.91(9)		C14	C23	1.47(12)
Np9	O57	1.81(6)		C16	C22	1.48(12)
Np10	Np8[2]	4.007(5)		C17	C18	1.41(11)
Np10	O4	1.85(7)		C18	C24	1.35(12)
Np10	O5	1.84(6)		C19	Np7[3]	2.88(9)
Np10	O31[2]	2.34(7)		C20	C22	1.58(13)
Np10	O37	2.46(6)		C22	C24	1.40(12)

[1]1+X,+Y,+Z; [2]+X,-1+Y,+Z; [3]-1/2+X,2-Y,-1/2+Z; [4]+X,1+Y,+Z; [5]-1+X,+Y,+Z; [6]1/2+X,2-Y,1/2+Z; [7]-1+X,1+Y,+Z; [8]1+X,-1+Y,+Z; [9]1/2+X,2-Y,-1/2+Z; [10]-1/2+X,2-Y,1/2+Z

II.12 U-La-I

Table 1 Crystal data and structure refinement for U-La-I.	
Identification code	U-La-I
Empirical formula	$C_{126}La_4N_{18}O_{123}U_6$
Formula weight	5717.26
Temperature/K	293(2)
Crystal system	triclinic
Space group	P1
a/Å	16.528
b/Å	16.945
c/Å	19.478
α/°	96.75
β/°	99.93
γ/°	118.22
Volume/Å^3	4608.1
Z	1
ρ_{calc}g/cm^3	2.060
μ/mm^{-1}	6.276
F(000)	2646.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.802 to 52.736

Index ranges	$-20 \leq h \leq 20$, $-21 \leq k \leq 21$, $-24 \leq l \leq 24$
Reflections collected	103453
Independent reflections	36862 [R_{int} = 0.0543, R_{sigma} = 0.0972]
Data/restraints/parameters	36862/3/1159
Goodness-of-fit on F^2	0.925
Final R indexes [I>=2σ (I)]	R_1 = 0.0556, wR_2 = 0.1395
Final R indexes [all data]	R_1 = 0.0860, wR_2 = 0.1580
Largest diff. peak/hole / e $Å^{-3}$	1.56/-1.58
Flack parameter	0.130(3)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for U-La-I. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	-4467.8(7)	-6707.9(7)	-7789.8(6)	24.6(3)
La1	-5640.2(12)	-3375.6(13)	-7889(1)	27.9(4)
O11W	-4850(30)	-3910(30)	-8720(20)	74(9)
O12W	-6980(18)	-4722(17)	-8924(13)	46(5)
O13W	-5610(20)	-2820(20)	-9046(15)	53(7)
O14W	-6980(20)	-2940(20)	-8208(18)	74(9)
O15W	-7010(20)	-4440(20)	-7366(15)	56(7)
O16W	-4880(20)	-1580(20)	-7607(16)	65(7)
O17W	-5410(20)	-2620(20)	-6577(18)	71(8)
O18W	-3830(20)	-2620(20)	-7302(16)	57(7)
U6	-10194.7(8)	-2106.7(7)	-3788.6(6)	26.2(3)
U3	-4542.5(7)	-300.9(7)	-4516.4(5)	23.3(3)
U2	33.2(7)	-8559.7(7)	-6983.6(6)	24.3(3)
La4	-9823.2(12)	-8127.9(12)	-2473.9(10)	28.2(4)
U5	-9880.9(7)	-4853.0(7)	-166.2(5)	24.0(3)
O41W	-10008(18)	-6714(18)	-2579(14)	46(6)
O42W	-11564(16)	-8573(16)	-3052(12)	42(5)
O43W	-9949(17)	-7968(17)	-3767(13)	43(5)
O44W	-8140(20)	-6853(19)	-2401(15)	41(6)
O45W	-10940(20)	-8960(20)	-1710(15)	54(6)
O46W	-8780(20)	-8380(20)	-1479(15)	54(7)
O47W	-8920(20)	-8820(20)	-3078(16)	57(7)
La3	-4349.8(12)	-6903.3(12)	-2442.1(10)	27.9(4)
U4	-4421.6(7)	-2998.7(7)	-979.9(6)	27.7(3)
O31W	-6060(20)	-7340(20)	-2641(17)	66(8)
O32W	-4430(20)	-5880(20)	-3277(15)	57(6)
O33W	-4730(20)	-7310(20)	-1276(18)	71(8)
O34W	-2820(30)	-6360(30)	-1530(20)	77(10)
O35W	-4310(20)	-8360(20)	-2315(15)	51(7)
O36W	-3045(18)	-6503(18)	-3037(14)	48(6)
La2	-8767.7(12)	-1881.0(12)	-6920.6(10)	29.4(4)
O21W	-7410(20)	-2260(20)	-6914(18)	73(8)
O22W	-7470(20)	-640(20)	-7388(15)	57(7)
O23W	-7440(19)	-711(18)	-5853(14)	50(6)
O24W	-8680(18)	-2632(18)	-5893(14)	49(6)

O25W	-9480(20)	-1390(20)	-5991(16)	54(7)
O26W	-10570(20)	-2630(20)	-7414(16)	55(7)
O27W	-9620(20)	-3672(19)	-7343(15)	47(6)
O28W	-8860(30)	-2470(30)	-8210(20)	71(9)
O1S	-10650(20)	-6400(20)	-3830(16)	63(7)
O2S	-3060(30)	-7260(20)	-4343(19)	65(9)
O3S	-2810(40)	300(40)	-590(30)	96(16)
O4S	-6846(19)	-6264(19)	-8860(15)	58(6)
O5S	-11180(20)	-1530(20)	-6745(17)	65(8)
O6S	-7410(20)	-8340(20)	-3874(17)	64(7)
O7S	-7360(20)	-6770(20)	-446(18)	65(8)
O8S	-6370(20)	-6350(20)	-1524(18)	65(8)
O9S	-6800(30)	-3010(30)	-5900(20)	80(11)
O10S	-9680(30)	-9890(30)	-1040(20)	84(10)
O11S	-7760(20)	-6240(20)	-3626(16)	61(7)
O12S	-5720(30)	-5260(30)	-3560(20)	89(11)
O13S	-8960(40)	-5690(40)	-4330(30)	117(16)
O14S	-3130(30)	-3660(30)	-7870(20)	94(11)
O15S	-11970(50)	-7490(50)	-2200(40)	150(20)
O16S	-11410(30)	-5330(30)	-4124(19)	79(9)
O17S	-7520(50)	830(60)	-5870(40)	160(30)
O18S	-5870(60)	-4360(60)	-4590(40)	190(30)
O19S	-7240(60)	-3640(60)	-4520(50)	210(30)
O20S	-1620(60)	2060(60)	-1000(50)	210(30)
O21S	-8410(60)	-1350(60)	-70(50)	240(30)
O22S	-8500(40)	-4350(40)	-6230(30)	135(17)
N1A	-3106(18)	-6867(18)	-8045(14)	30(5)
C2A	-3170(20)	-7690(20)	-8160(17)	32(6)
C3A	-2440(30)	-7830(30)	-8330(20)	53(8)
C4A	-1640(30)	-7070(30)	-8320(20)	61(9)
C5A	-1530(30)	-6190(30)	-8190(20)	42(8)
C6A	-2250(20)	-6110(20)	-8056(18)	30(7)
C7A	-4130(20)	-8470(20)	-8132(18)	34(7)
C8A	-2290(30)	-5220(20)	-7880(20)	37(8)
O71A	-4715(17)	-8221(17)	-8027(13)	44(5)
O72A	-4240(20)	-9230(20)	-8172(16)	54(7)
O81A	-3020(17)	-5289(16)	-7763(13)	35(5)
O82A	-1560(20)	-4510(20)	-7850(16)	46(7)
N1B	-4151(18)	-5578(18)	-6641(14)	26(5)
C2B	-4490(20)	-4990(20)	-6646(17)	29(6)
C3B	-4360(30)	-4380(30)	-6050(20)	33(8)
C4B	-3860(30)	-4420(30)	-5380(20)	45(9)
C5B	-3550(30)	-5040(30)	-5380(20)	41(8)
C6B	-3700(20)	-5600(20)	-6003(17)	37(7)
C7B	-5020(20)	-5090(20)	-7397(18)	27(7)
C8B	-3350(20)	-6250(20)	-6081(19)	32(7)
O71B	-5101(16)	-5660(16)	-7911(13)	31(5)
O72B	-5350(20)	-4560(20)	-7474(16)	38(7)

O81B	-3583(17)	-6748(16)	-6712(13)	37(5)
O82B	-2920(20)	-6330(20)	-5532(17)	60(7)
N1C	1727(17)	-7620(17)	-6254(13)	34(5)
C2C	1970(20)	-7510(20)	-5521(16)	28(6)
C3C	2910(30)	-7000(30)	-5110(20)	37(8)
C4C	3610(30)	-6560(30)	-5430(20)	38(9)
C5C	3340(30)	-6680(30)	-6210(20)	48(8)
C6C	2450(20)	-7180(20)	-6558(17)	34(6)
C7C	1140(20)	-8030(20)	-5263(17)	38(7)
C8C	2070(20)	-7320(20)	-7351(19)	38(7)
O71C	318(16)	-8473(16)	-5724(13)	36(5)
O72C	1270(20)	-7990(20)	-4574(15)	46(7)
O81C	1191(16)	-7847(16)	-7605(12)	40(5)
O82C	2670(20)	-6940(20)	-7699(16)	58(7)
N1D	-1288(18)	-8383(18)	-6611(14)	32(5)
C2D	-2090(20)	-9140(20)	-6617(17)	26(7)
C3D	-2870(30)	-9090(30)	-6480(20)	42(8)
C4D	-2760(30)	-8200(30)	-6300(20)	52(9)
C5D	-1890(30)	-7420(30)	-6280(20)	50(8)
C6D	-1190(20)	-7590(20)	-6471(17)	31(7)
C7D	-2160(20)	-10040(20)	-6812(18)	33(7)
C8D	-240(30)	-6800(20)	-6480(19)	37(7)
O71D	-1384(17)	-9963(16)	-6949(13)	32(5)
O72D	-2850(20)	-10760(20)	-6845(16)	50(7)
O81D	331(17)	-7055(16)	-6645(13)	42(5)
O82D	-50(20)	-5990(20)	-6328(16)	70(7)
N1E	-344(18)	-9719(18)	-8119(14)	26(5)
C2E	-30(20)	-10300(20)	-8101(17)	25(6)
C3E	-130(30)	-10870(30)	-8720(20)	48(8)
C4E	-630(30)	-10880(30)	-9380(20)	56(9)
C5E	-950(30)	-10220(30)	-9390(20)	44(8)
C6E	-800(20)	-9670(20)	-8725(17)	40(7)
C7E	510(20)	-10250(20)	-7361(18)	31(7)
C8E	-1140(20)	-8970(20)	-8661(19)	42(7)
O71E	573(16)	-9637(16)	-6874(12)	38(5)
O72E	860(20)	-10740(20)	-7297(16)	41(7)
O81E	-902(17)	-8539(17)	-8010(13)	37(5)
O82E	-1570(20)	-8880(20)	-9188(16)	59(7)
N1F	-5086(18)	646(17)	-5145(13)	27(5)
C2F	-5230(20)	540(20)	-5881(17)	25(6)
C3F	-5430(30)	1100(30)	-6240(20)	46(8)
C4F	-5460(30)	1830(30)	-5840(20)	53(9)
C5F	-5370(30)	1930(30)	-5100(20)	51(8)
C6F	-5160(20)	1330(20)	-4777(17)	25(6)
C7F	-5160(20)	-290(20)	-6206(17)	33(6)
C8F	-4960(30)	1420(20)	-3987(19)	26(7)
O71F	-4910(16)	-685(16)	-5777(12)	34(5)
O72F	-5390(20)	-500(20)	-6866(16)	55(7)

O81F	-4688(16)	862(16)	-3767(12)	38(5)
O82F	-5090(20)	1960(20)	-3613(16)	48(7)
N1G	-3242(18)	-538(18)	-4836(14)	32(5)
C2G	-3360(20)	-1400(20)	-4972(17)	27(6)
C3G	-2670(30)	-1560(30)	-5130(20)	43(8)
C4G	-1840(30)	-820(30)	-5180(20)	55(9)
C5G	-1690(30)	100(30)	-5030(20)	36(8)
C6G	-2420(20)	190(20)	-4867(17)	36(6)
C7G	-4330(20)	-2140(20)	-4891(18)	29(7)
C8G	-2410(30)	1090(20)	-4672(19)	32(8)
O71G	-4863(17)	-1824(16)	-4755(13)	36(5)
O72G	-4500(20)	-2940(20)	-4981(16)	47(7)
O81G	-3148(17)	1049(16)	-4587(13)	35(5)
O82G	-1650(20)	1820(20)	-4640(17)	46(7)
N1H	-5250(17)	-910(17)	-3518(13)	27(5)
C2H	-4710(20)	-750(20)	-2866(16)	28(6)
C3H	-5040(30)	-1040(30)	-2300(20)	33(8)
C4H	-6020(30)	-1510(30)	-2370(20)	47(9)
C5H	-6640(30)	-1730(30)	-3070(20)	49(8)
C6H	-6180(20)	-1370(20)	-3621(17)	35(6)
C7H	-3650(20)	-220(20)	-2832(17)	33(6)
C8H	-6770(20)	-1540(20)	-4380(18)	32(7)
O71H	-3449(17)	21(16)	-3427(12)	33(5)
O72H	-3060(20)	0(20)	-2265(16)	43(7)
O81H	-6223(16)	-1130(16)	-4780(12)	35(5)
O82H	-7640(20)	-1980(20)	-4532(16)	48(7)
N1I	-4007(18)	-1849(18)	160(14)	28(5)
C2I	-4340(20)	-1290(20)	151(17)	35(6)
C3I	-4100(30)	-600(30)	760(20)	37(8)
C4I	-3470(30)	-520(30)	1370(20)	38(9)
C5I	-3080(30)	-1110(30)	1350(20)	41(8)
C6I	-3410(20)	-1770(20)	735(17)	29(7)
C7I	-5000(20)	-1430(20)	-532(18)	35(7)
C8I	-3100(20)	-2470(20)	667(19)	32(7)
O71I	-5161(16)	-2104(16)	-1026(13)	41(5)
O72I	-5380(20)	-960(20)	-613(16)	60(7)
O81I	-3471(17)	-3042(16)	51(13)	43(5)
O82I	-2530(20)	-2480(20)	1183(16)	48(7)
N1J	-3102(18)	-3126(17)	-1399(14)	29(5)
C2J	-2310(20)	-2340(20)	-1384(17)	36(6)
C3J	-1560(30)	-2390(30)	-1610(20)	39(8)
C4J	-1650(30)	-3220(30)	-1790(20)	48(9)
C5J	-2410(30)	-4020(30)	-1770(20)	45(8)
C6J	-3150(20)	-3930(20)	-1577(17)	37(7)
C7J	-2340(20)	-1480(20)	-1168(17)	32(7)
C8J	-4060(30)	-4740(20)	-1496(19)	27(7)
O71J	-3087(16)	-1603(16)	-1001(13)	42(5)
O72J	-1640(20)	-730(20)	-1180(15)	57(7)

O81J	-4663(16)	-4537(16)	-1325(13)	39(5)
O82J	-4200(20)	-5540(20)	-1684(17)	52(7)
N1K	-6147(17)	-3951(17)	-1709(13)	36(5)
C2K	-6810(20)	-4400(20)	-1402(16)	35(6)
C3K	-7800(30)	-4850(30)	-1760(20)	40(8)
C4K	-8000(30)	-4730(30)	-2460(20)	41(9)
C5K	-7290(30)	-4230(30)	-2780(20)	49(8)
C6K	-6340(20)	-3850(20)	-2366(17)	34(6)
C7K	-6510(20)	-4400(20)	-657(17)	36(7)
C8K	-5510(20)	-3280(20)	-2654(19)	37(7)
O71K	-5578(16)	-3935(16)	-374(12)	43(5)
O72K	-7080(20)	-4870(20)	-335(15)	53(7)
O81K	-4698(16)	-2983(16)	-2177(12)	39(5)
O82K	-5600(20)	-3130(20)	-3235(16)	61(7)
N1L	-11298(18)	-4804(18)	116(14)	40(5)
C2L	-11300(20)	-4010(20)	202(17)	41(6)
C3L	-12070(30)	-3940(30)	320(20)	63(8)
C4L	-12830(30)	-4720(30)	350(20)	68(9)
C5L	-12890(30)	-5580(30)	290(20)	57(8)
C6L	-12080(20)	-5580(20)	145(17)	40(7)
C7L	-10400(20)	-3200(20)	166(17)	47(7)
C8L	-12000(30)	-6430(20)	-20(20)	40(8)
O71L	-9748(16)	-3403(16)	59(12)	47(5)
O72L	-10300(20)	-2450(20)	245(16)	76(7)
O81L	-11221(17)	-6278(16)	-140(13)	40(5)
O82L	-12680(20)	-7160(20)	4(16)	70(7)
N1M	-9156(17)	-3988(17)	-1075(13)	25(5)
C2M	-9700(20)	-4100(20)	-1699(16)	33(6)
C3M	-9380(30)	-3590(30)	-2170(20)	43(8)
C4M	-8410(30)	-2880(30)	-1990(20)	57(9)
C5M	-7810(30)	-2780(30)	-1340(20)	52(8)
C6M	-8260(20)	-3320(20)	-888(17)	33(6)
C7M	-10710(20)	-4830(20)	-1827(17)	33(6)
C8M	-7730(20)	-3280(20)	-166(19)	48(7)
O71M	-10950(17)	-5165(16)	-1303(13)	42(5)
O72M	-11300(20)	-5040(20)	-2419(16)	54(7)
O81M	-8214(16)	-3817(16)	203(12)	41(5)
O82M	-6830(20)	-2700(20)	75(16)	66(7)
N1N	-9326(18)	-5872(17)	376(14)	27(5)
C2N	-9200(20)	-5820(20)	1066(17)	25(6)
C3N	-9070(30)	-6450(30)	1400(20)	34(8)
C4N	-9110(30)	-7180(30)	940(20)	50(9)
C5N	-9210(30)	-7230(30)	230(20)	40(8)
C6N	-9360(20)	-6550(20)	-49(17)	26(7)
C7N	-9190(20)	-5000(20)	1485(18)	21(7)
C8N	-9500(20)	-6500(20)	-830(19)	42(7)
O71N	-9444(17)	-4549(16)	1108(12)	42(5)
O72N	-8960(20)	-4810(20)	2157(16)	51(7)

O81N	-9680(16)	-5900(16)	-984(12)	32(5)
O82N	-9470(20)	-7090(20)	-1251(16)	50(7)
N1O	-10420(18)	-3274(18)	-4843(14)	28(5)
C2O	-10010(20)	-3760(20)	-4783(17)	37(6)
C3O	-10170(30)	-4470(30)	-5320(20)	42(8)
C4O	-10830(30)	-4660(30)	-5990(20)	48(9)
C5O	-11270(30)	-4140(30)	-6060(20)	34(8)
C6O	-11050(20)	-3450(20)	-5468(17)	36(7)
C7O	-9300(20)	-3470(20)	-4054(17)	24(6)
C8O	-11490(20)	-2820(20)	-5447(19)	30(7)
O71O	-9280(16)	-2836(16)	-3606(13)	38(5)
O72O	-8820(20)	-3850(20)	-3944(15)	53(7)
O81O	-11227(16)	-2275(16)	-4853(12)	37(5)
O82O	-12020(20)	-2880(20)	-5981(16)	50(7)
N1P	-8547(17)	-904(17)	-3028(13)	29(5)
C2P	-8360(20)	-780(20)	-2340(16)	47(6)
C3P	-7460(30)	-180(30)	-1883(19)	50(8)
C4P	-6730(30)	330(30)	-2220(20)	64(9)
C5P	-6970(30)	200(30)	-2980(20)	53(8)
C6P	-7850(20)	-360(20)	-3354(17)	41(6)
C7P	-9190(20)	-1370(20)	-2090(17)	39(6)
C8P	-8190(20)	-560(20)	-4132(18)	40(7)
O71P	-9922(16)	-1923(16)	-2540(12)	41(5)
O72P	-9110(20)	-1260(20)	-1407(16)	63(7)
O81P	-9080(16)	-1179(16)	-4414(12)	41(5)
O82P	-7680(20)	-90(20)	-4484(16)	62(7)
N1Q	-6107(17)	-7751(17)	-8654(13)	30(5)
C2Q	-6810(20)	-8310(20)	-8393(16)	38(6)
C3Q	-7700(30)	-8960(30)	-8870(20)	53(8)
C4Q	-7890(30)	-9040(30)	-9610(20)	76(9)
C5Q	-7080(30)	-8410(30)	-9870(20)	59(8)
C6Q	-6220(20)	-7750(20)	-9334(17)	33(6)
C7Q	-6550(20)	-8200(20)	-7603(17)	35(7)
C8Q	-5330(20)	-7060(20)	-9515(19)	40(7)
O71Q	-5732(16)	-7560(16)	-7285(12)	33(5)
O72Q	-7130(20)	-8740(20)	-7335(16)	52(7)
O81Q	-4609(17)	-6603(16)	-9005(13)	49(5)
O82Q	-5390(20)	-7010(20)	-10147(16)	78(7)
N1R	-11639(18)	-2170(17)	-3445(14)	25(5)
C2R	-11720(20)	-1430(20)	-3287(16)	40(6)
C3R	-12530(30)	-1440(30)	-3160(20)	41(8)
C4R	-13310(30)	-2290(30)	-3170(20)	52(9)
C5R	-13250(30)	-3120(30)	-3330(20)	52(8)
C6R	-12380(20)	-2980(20)	-3422(17)	35(7)
C7R	-10820(20)	-560(20)	-3261(17)	37(6)
C8R	-12220(20)	-3810(20)	-3598(19)	40(7)
O71R	-10172(16)	-648(16)	-3461(12)	41(5)
O72R	-10800(20)	190(20)	-3051(15)	55(7)

O81R	-11402(17)	-3565(16)	-3741(13)	37(5)
O82R	-12830(20)	-4600(20)	-3611(16)	50(7)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U-La-I. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	22.8(5)	23.8(5)	29.4(6)	2.1(4)	6.5(4)	14.4(4)
La1	26.7(8)	32.8(9)	30.9(9)	7.8(7)	6.2(7)	20.6(7)
U6	26.8(5)	23.5(5)	31.8(6)	3.4(4)	10.8(4)	14.9(4)
U3	24.5(5)	26.1(5)	24.6(5)	5.7(4)	8.8(4)	16.0(4)
U2	26.5(5)	24.5(5)	26.3(5)	3.4(4)	7.1(4)	16.8(4)
La4	26.3(8)	24.5(8)	32.6(9)	1.3(6)	8.0(6)	12.9(6)
U5	23.5(5)	23.9(5)	26.5(6)	4.9(4)	6.6(4)	13.7(4)
La3	26.8(8)	23.6(8)	30.2(9)	-1.2(6)	6.7(6)	12.1(6)
U4	26.9(5)	28.3(6)	27.1(6)	0.1(4)	9.0(4)	14.0(5)
La2	25.6(8)	28.3(8)	35.7(10)	5.2(7)	2.5(7)	17.0(7)

Table 4 Bond Lengths for U-La-I.

Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å	Atom	Atom	Length/Å
U1	N1A	2.51(3)	C3F	C4F	1.39(6)	U4	N1K	2.54(2)	C7L	O71L	1.32(4)
U1	O71A	2.37(2)	C4F	C5F	1.40(6)	U4	O71K	2.43(2)	C7L	O72L	1.18(4)
U1	O81A	2.45(2)	C5F	C6F	1.39(5)	U4	O81K	2.30(2)	C8L	O81L	1.26(4)
U1	N1B	2.57(3)	C6F	C8F	1.49(5)	La2	O21W	2.60(3)	C8L	O82L	1.23(5)
U1	O71B	2.46(2)	C7F	O71F	1.27(4)	La2	O22W	2.59(3)	N1M	C2M	1.32(4)
U1	O81B	2.37(2)	C7F	O72F	1.23(4)	La2	O23W	2.53(3)	N1M	C6M	1.32(4)
U1	N1Q	2.55(2)	C8F	O81F	1.30(4)	La2	O24W	2.51(3)	C2M	C3M	1.34(5)
U1	O71Q	2.37(2)	C8F	O82F	1.22(5)	La2	O25W	2.59(3)	C2M	C7M	1.49(4)
U1	O81Q	2.37(2)	O82F	$La3^4$	2.49(3)	La2	O26W	2.56(3)	C3M	C4M	1.41(5)
La1	O11W	2.58(4)	N1G	C2G	1.37(4)	La2	O27W	2.61(3)	C4M	C5M	1.40(5)
La1	O12W	2.60(3)	N1G	C6G	1.36(4)	La2	O28W	2.55(4)	C5M	C6M	1.39(5)
La1	O13W	2.54(3)	C2G	C3G	1.37(5)	La2	$O72E^2$	2.44(3)	C6M	C8M	1.50(5)
La1	O14W	2.64(4)	C2G	C7G	1.55(4)	N1A	C2A	1.34(4)	C7M	O71M	1.26(4)
La1	O15W	2.60(3)	C3G	C4G	1.39(6)	N1A	C6A	1.39(4)	C7M	O72M	1.26(4)
La1	O16W	2.63(3)	C4G	C5G	1.45(6)	C2A	C3A	1.42(5)	C8M	O81M	1.28(4)
La1	O17W	2.60(4)	C5G	C6G	1.36(5)	C2A	C7A	1.52(4)	C8M	O82M	1.29(4)
La1	O18W	2.60(3)	C6G	C8G	1.52(5)	C3A	C4A	1.34(6)	N1N	C2N	1.31(4)
La1	O72B	2.46(3)	C7G	O71G	1.28(4)	C4A	C5A	1.39(6)	N1N	C6N	1.31(4)
U6	N1O	2.52(3)	C7G	O72G	1.22(4)	C5A	C6A	1.34(5)	C2N	C3N	1.39(5)
U6	O71O	2.37(2)	C8G	O81G	1.23(4)	C6A	C8A	1.54(5)	C2N	C7N	1.53(5)
U6	O81O	2.34(2)	C8G	O82G	1.25(5)	C7A	O71A	1.26(4)	C3N	C4N	1.41(6)
U6	N1P	2.53(2)	N1H	C2H	1.33(4)	C7A	O72A	1.22(5)	C4N	C5N	1.36(6)
U6	O71P	2.35(2)	N1H	C6H	1.31(4)	C8A	O81A	1.22(4)	C5N	C6N	1.43(5)
U6	O81P	2.42(2)	C2H	C3H	1.34(5)	C8A	O82A	1.22(5)	C6N	C8N	1.52(5)
U6	N1R	2.55(3)	C2H	C7H	1.53(4)	N1B	C2B	1.36(4)	C7N	O71N	1.27(4)
U6	O71R	2.46(2)	C3H	C4H	1.41(5)	N1B	C6B	1.35(4)	C7N	O72N	1.26(4)

U6	O81R	2.36(2)		C4H	C5H	1.44(6)		C2B	C3B	1.38(5)		C8N	O81N	1.24(4)
U3	N1F	2.51(3)		C5H	C6H	1.45(5)		C2B	C7B	1.51(4)		C8N	O82N	1.24(5)
U3	O71F	2.36(2)		C6H	C8H	1.54(5)		C3B	C4B	1.44(6)		N1O	C2O	1.29(4)
U3	O81F	2.44(2)		C7H	O71H	1.32(4)		C4B	C5B	1.37(6)		N1O	C6O	1.36(4)
U3	N1G	2.53(3)		C7H	O72H	1.22(4)		C5B	C6B	1.36(5)		C2O	C3O	1.40(5)
U3	O71G	2.35(2)		C8H	O81H	1.29(4)		C6B	C8B	1.47(5)		C2O	C7O	1.53(4)
U3	O81G	2.40(2)		C8H	O82H	1.24(4)		C7B	O71B	1.25(4)		C3O	C4O	1.45(6)
U3	N1H	2.51(2)		N1I	C2I	1.30(4)		C7B	O72B	1.27(5)		C4O	C5O	1.39(6)
U3	O71H	2.35(2)		N1I	C6I	1.30(4)		C8B	O81B	1.29(4)		C5O	C6O	1.40(5)
U3	O81H	2.37(2)		C2I	C3I	1.42(5)		C8B	O82B	1.24(5)		C6O	C8O	1.54(5)
U2	N1C	2.50(2)		C2I	C7I	1.48(4)		N1C	C2C	1.38(4)		C7O	O71O	1.28(4)
U2	O71C	2.39(2)		C3I	C4I	1.39(5)		N1C	C6C	1.36(4)		C7O	O72O	1.25(4)
U2	O81C	2.35(2)		C4I	C5I	1.42(6)		C2C	C3C	1.39(5)		C8O	O81O	1.26(4)
U2	N1D	2.55(3)		C5I	C6I	1.36(5)		C2C	C7C	1.45(4)		C8O	O82O	1.20(4)
U2	O71D	2.44(2)		C6I	C8I	1.49(5)		C3C	C4C	1.36(6)		N1P	C2P	1.29(4)
U2	O81D	2.34(2)		C7I	O71I	1.29(4)		C4C	C5C	1.47(6)		N1P	C6P	1.40(4)
U2	N1E	2.55(3)		C7I	O72I	1.25(5)		C5C	C6C	1.30(5)		C2P	C3P	1.40(5)
U2	O71E	2.40(2)		C8I	O81I	1.29(4)		C6C	C8C	1.51(5)		C2P	C7P	1.47(4)
U2	O81E	2.32(2)		C8I	O82I	1.27(5)		C7C	O71C	1.29(4)		C3P	C4P	1.43(5)
La4	O41W	2.58(3)		N1J	C2J	1.35(4)		C7C	O72C	1.31(4)		C4P	C5P	1.43(6)
La4	O42W	2.60(2)		N1J	C6J	1.33(4)		C8C	O81C	1.25(4)		C5P	C6P	1.31(5)
La4	O43W	2.55(2)		C2J	C3J	1.42(5)		C8C	O82C	1.26(5)		C6P	C8P	1.46(5)
La4	O44W	2.55(3)		C2J	C7J	1.49(5)		N1D	C2D	1.34(4)		C7P	O71P	1.22(4)
La4	O45W	2.56(3)		C3J	C4J	1.35(6)		N1D	C6D	1.27(4)		C7P	O72P	1.30(4)
La4	O46W	2.58(3)		C4J	C5J	1.35(5)		C2D	C3D	1.39(5)		C8P	O81P	1.30(4)
La4	O47W	2.63(3)		C5J	C6J	1.41(5)		C2D	C7D	1.47(5)		C8P	O82P	1.23(5)
La4	O82N	2.58(3)		C6J	C8J	1.53(5)		C3D	C4D	1.44(6)		N1Q	C2Q	1.34(4)
La4	O72R[1]	2.50(3)		C7J	O71J	1.26(4)		C4D	C5D	1.41(6)		N1Q	C6Q	1.30(4)
U5	N1L	2.53(3)		C7J	O72J	1.25(4)		C5D	C6D	1.40(5)		C2Q	C3Q	1.41(5)
U5	O71L	2.34(2)		C8J	O81J	1.28(4)		C6D	C8D	1.51(5)		C2Q	C7Q	1.49(4)
U5	O81L	2.40(2)		C8J	O82J	1.26(5)		C7D	O71D	1.30(4)		C3Q	C4Q	1.39(6)
U5	N1M	2.53(2)		N1K	C2K	1.30(4)		C7D	O72D	1.20(5)		C4Q	C5Q	1.48(6)
U5	O71M	2.41(2)		N1K	C6K	1.31(4)		C8D	O81D	1.28(4)		C5Q	C6Q	1.44(5)
U5	O81M	2.37(2)		C2K	C3K	1.43(5)		C8D	O82D	1.23(5)		C6Q	C8Q	1.52(5)
U5	N1N	2.56(3)		C2K	C7K	1.45(4)		N1E	C2E	1.31(4)		C7Q	O71Q	1.24(4)
U5	O71N	2.38(2)		C3K	C4K	1.41(6)		N1E	C6E	1.32(4)		C7Q	O72Q	1.22(4)
U5	O81N	2.42(2)		C4K	C5K	1.37(6)		C2E	C3E	1.39(5)		C8Q	O81Q	1.24(4)
La3	O31W	2.50(3)		C5K	C6K	1.41(5)		C2E	C7E	1.53(4)		C8Q	O82Q	1.24(5)
La3	O32W	2.55(3)		C6K	C8K	1.51(5)		C3E	C4E	1.41(6)		N1R	C2R	1.33(4)
La3	O33W	2.55(3)		C7K	O71K	1.32(4)		C4E	C5E	1.43(6)		N1R	C6R	1.36(4)
La3	O34W	2.50(4)		C7K	O72K	1.24(4)		C5E	C6E	1.42(5)		C2R	C3R	1.39(5)
La3	O35W	2.54(3)		C8K	O81K	1.32(4)		C6E	C8E	1.53(5)		C2R	C7R	1.50(4)
La3	O36W	2.47(3)		C8K	O82K	1.18(5)		C7E	O71E	1.27(4)		C3R	C4R	1.41(5)
La3	O82F[1]	2.49(3)		N1L	C2L	1.34(4)		C7E	O72E	1.23(4)		C4R	C5R	1.45(6)
La3	O82J	2.47(3)		N1L	C6L	1.36(4)		C8E	O81E	1.28(4)		C5R	C6R	1.39(5)
U4	N1I	2.53(3)		C2L	C3L	1.38(5)		C8E	O82E	1.21(5)		C6R	C8R	1.57(5)
U4	O71I	2.35(2)		C2L	C7L	1.49(4)		O72E	La2[3]	2.44(3)		C7R	O71R	1.27(4)
U4	O81I	2.36(2)		C3L	C4L	1.34(5)		N1F	C2F	1.39(4)		C7R	O72R	1.27(4)

U4	N1J	2.55(3)		C4L	C5L	1.41(6)		N1F	C6F	1.36(4)		C8R	O81R	1.30(4)
U4	O71J	2.36(2)		C5L	C6L	1.40(5)		C2F	C3F	1.37(5)		C8R	O82R	1.23(5)
U4	O81J	2.43(2)		C6L	C8L	1.51(5)		C2F	C7F	1.53(5)		O72R	La4[4]	2.50(3)

[1]+X,-1+Y,+Z; [2]-1+X,1+Y,+Z; [3]1+X,-1+Y,+Z; [4]+X,1+Y,+Z

II.13 U-Ce-I

Table 1 Crystal data and structure refinement for U-Ce-I.	
Identification code	U-Ce-I
Empirical formula	$C_{126}Ce_4N_{18}O_{120}U_6$
Formula weight	5674.10
Temperature/K	293(2)
Crystal system	triclinic
Space group	P1
a/Å	16.487
b/Å	16.889
c/Å	19.500
α/°	96.80
β/°	100.18
γ/°	118.57
Volume/Å^3	4562.3
Z	1
ρ_{calc}g/cm^3	2.065
μ/mm^{-1}	6.398
F(000)	2626.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.824 to 56.752
Index ranges	-21 ≤ h ≤ 21, -22 ≤ k ≤ 22, -25 ≤ l ≤ 25
Reflections collected	210312
Independent reflections	44777 [R_{int} = 0.0547, R_{sigma} = 0.0623]
Data/restraints/parameters	44777/3/2372
Goodness-of-fit on F^2	1.113
Final R indexes [I>=2σ (I)]	R_1 = 0.0542, wR_2 = 0.1525
Final R indexes [all data]	R_1 = 0.0736, wR_2 = 0.1642
Largest diff. peak/hole / e Å^{-3}	1.66/-1.31
Flack parameter	0.435(2)

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Ce-I. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	-4481.2(6)	-6710.8(6)	-7807.8(5)	24.0(2)
Ce1	-5647.2(10)	-3379.3(10)	-7895.6(8)	27.9(3)
O11W	-4920(20)	-3940(20)	-8790(20)	69(8)
O12W	-6972(13)	-4708(17)	-8901(10)	54(6)
O13W	-5586(18)	-2770(20)	-9012(15)	66(8)

O14W	-7010(20)	-3000(30)	-8200(20)	87(10)
O15W	-6998(17)	-4432(18)	-7382(12)	55(6)
O16W	-4880(20)	-1580(20)	-7652(17)	71(7)
O17W	-5450(20)	-2660(20)	-6590(14)	67(9)
O18W	-3873(16)	-2642(18)	-7352(17)	58(7)
U6	-10175.2(7)	-2096.9(6)	-3789.3(5)	27.8(2)
U3	-4545.3(6)	-309.7(6)	-4529.4(4)	23.2(2)
U2	43.2(6)	-8552.7(6)	-6965.7(4)	24.0(2)
Ce4	-9850.6(11)	-8113.4(11)	-2463.2(8)	32.8(3)
U5	-9889.4(6)	-4852.0(6)	-158.0(4)	24.2(2)
O41W	-9997(18)	-6691(15)	-2566(14)	52(6)
O42W	-11561(17)	-8540(20)	-3055(15)	52(6)
O43W	-9955(14)	-7967(17)	-3740(10)	45(5)
O44W	-8199(19)	-6880(20)	-2381(15)	56(6)
O45W	-10940(20)	-8999(19)	-1708(16)	61(7)
O46W	-8778(18)	-8370(18)	-1502(13)	50(5)
O47W	-8910(30)	-8750(30)	-3080(30)	87(11)
Ce3	-4361.4(11)	-6918.3(10)	-2447.7(8)	29.8(3)
U4	-4415.7(7)	-3008.4(6)	-976.6(5)	29.0(2)
O31W	-6030(20)	-7330(20)	-2609(16)	67(8)
O32W	-4440(20)	-5900(20)	-3316(16)	61(7)
O33W	-4680(20)	-7330(20)	-1270(12)	64(7)
O34W	-2840(20)	-6380(30)	-1568(18)	87(14)
O35W	-4290(20)	-8354(18)	-2297(13)	48(6)
O36W	-3045(17)	-6510(20)	-3038(12)	58(6)
Ce2	-8765.5(10)	-1869.6(10)	-6915.9(8)	29.5(3)
O21W	-7440(20)	-2250(20)	-6914(19)	73(9)
O22W	-7450(20)	-620(20)	-7388(16)	57(7)
O23W	-7458(19)	-742(18)	-5888(16)	58(6)
O24W	-8699(18)	-2622(16)	-5905(14)	53(6)
O25W	-9473(19)	-1380(20)	-5985(11)	55(7)
O26W	-10544(17)	-2614(19)	-7453(19)	63(8)
O27W	-9598(17)	-3643(16)	-7302(17)	62(7)
O28W	-8890(30)	-2470(20)	-8191(19)	76(10)
O1S	-10680(30)	-6400(30)	-3810(19)	79(9)
O2S	-3070(30)	-7240(30)	-4330(20)	80(10)
O3S	-2660(40)	340(40)	-550(30)	114(18)
O4S	-6867(18)	-6274(18)	-8886(13)	53(5)
O5S	-11210(20)	-1550(20)	-6766(18)	70(8)
O6S	-7390(30)	-8370(30)	-3860(20)	81(9)
O7S	-7430(20)	-6790(20)	-463(16)	61(7)
O8S	-6360(20)	-6390(20)	-1509(15)	60(6)
O9S	-6790(30)	-3040(30)	-5900(20)	89(12)
O10S	-9690(30)	-9930(30)	-1070(20)	90(10)
O11S	-7770(20)	-6250(20)	-3594(17)	63(7)
O12S	-5750(30)	-5250(30)	-3580(20)	84(12)
O13S	-8950(40)	-5670(40)	-4340(30)	127(16)
O14S	-3190(20)	-3710(20)	-7976(17)	71(7)

O15S	-11390(30)	-5290(30)	-4130(20)	92(10)
O16S	-8580(40)	-4380(40)	-6230(30)	170(20)
O17S	-5880(50)	-4300(50)	-4530(40)	180(20)
O18S	-7560(50)	-9080(50)	-5940(40)	130(30)
O19S	-12030(60)	-7390(60)	-2310(50)	200(30)
N1A	-3100(17)	-6872(16)	-8063(12)	34(4)
C2A	-3200(20)	-7706(19)	-8182(14)	35(5)
C3A	-2460(20)	-7830(20)	-8322(19)	49(7)
C4A	-1650(30)	-7090(30)	-8340(20)	51(9)
C5A	-1510(30)	-6180(30)	-8160(20)	34(7)
C6A	-2280(20)	-6130(20)	-8063(15)	31(5)
C7A	-4150(20)	-8450(20)	-8135(16)	42(6)
C8A	-2280(20)	-5210(20)	-7907(18)	33(7)
O71A	-4755(16)	-8236(15)	-8072(13)	44(5)
O72A	-4230(20)	-9243(17)	-8169(17)	65(7)
O81A	-3017(15)	-5278(14)	-7782(13)	34(4)
O82A	-1550(20)	-4501(18)	-7886(18)	50(7)
N1B	-4149(17)	-5575(16)	-6657(12)	31(4)
C2B	-4500(20)	-4981(18)	-6683(15)	27(5)
C3B	-4390(30)	-4390(20)	-6073(18)	48(7)
C4B	-3900(30)	-4410(30)	-5380(19)	46(9)
C5B	-3570(30)	-5060(20)	-5384(17)	37(7)
C6B	-3700(20)	-5610(20)	-6039(15)	35(5)
C7B	-5020(20)	-5060(20)	-7433(17)	30(6)
C8B	-3360(20)	-6260(20)	-6121(17)	32(6)
O71B	-5075(16)	-5639(15)	-7935(11)	31(4)
O72B	-5390(20)	-4567(19)	-7493(14)	37(6)
O81B	-3570(16)	-6727(15)	-6738(11)	43(4)
O82B	-2950(20)	-6370(20)	-5551(14)	57(7)
N1C	1773(16)	-7587(16)	-6209(11)	24(4)
C2C	1983(19)	-7500(19)	-5517(13)	36(5)
C3C	2920(20)	-6990(20)	-5071(17)	42(7)
C4C	3640(20)	-6570(30)	-5400(20)	58(9)
C5C	3380(20)	-6620(20)	-6161(17)	49(7)
C6C	2470(20)	-7100(20)	-6526(14)	35(5)
C7C	1130(20)	-8040(20)	-5241(15)	32(5)
C8C	2120(20)	-7260(20)	-7311(16)	42(6)
O71C	321(15)	-8474(16)	-5692(11)	36(4)
O72C	1255(19)	-8010(20)	-4571(12)	49(7)
O81C	1204(14)	-7826(15)	-7586(10)	34(4)
O82C	2684(18)	-6870(20)	-7642(14)	68(7)
N1D	-1275(16)	-8381(16)	-6601(12)	27(4)
C2D	-2080(20)	-9120(20)	-6618(15)	24(5)
C3D	-2870(20)	-9070(30)	-6480(19)	52(7)
C4D	-2740(30)	-8180(30)	-6310(20)	56(9)
C5D	-1860(20)	-7410(20)	-6262(19)	52(7)
C6D	-1160(20)	-7540(20)	-6446(15)	39(5)
C7D	-2120(20)	-10030(20)	-6806(16)	31(6)

C8D	-200(20)	-6770(20)	-6465(17)	43(6)
O71D	-1368(15)	-9973(14)	-6940(13)	34(4)
O72D	-2871(19)	-10753(18)	-6862(17)	43(7)
O81D	350(15)	-7043(14)	-6609(12)	43(4)
O82D	-10(20)	-5979(17)	-6337(18)	68(7)
N1E	-314(16)	-9695(16)	-8095(12)	28(4)
C2E	10(20)	-10286(19)	-8096(15)	34(5)
C3E	-110(30)	-10890(20)	-8723(18)	40(7)
C4E	-620(30)	-10850(30)	-9342(19)	58(9)
C5E	-950(30)	-10220(20)	-9379(17)	50(7)
C6E	-770(20)	-9680(20)	-8725(15)	31(5)
C7E	520(20)	-10220(20)	-7375(17)	32(6)
C8E	-1060(20)	-8930(20)	-8658(17)	41(6)
O71E	585(16)	-9636(16)	-6869(11)	36(4)
O72E	870(20)	-10728(19)	-7279(15)	50(6)
O81E	-879(17)	-8509(15)	-8007(11)	35(4)
O82E	-1550(20)	-8850(20)	-9176(13)	50(7)
N1F	-5082(16)	654(15)	-5175(11)	23(4)
C2F	-5224(19)	558(19)	-5867(14)	29(5)
C3F	-5420(30)	1110(20)	-6242(18)	51(7)
C4F	-5430(30)	1860(30)	-5840(20)	50(8)
C5F	-5350(30)	1960(20)	-5089(17)	48(7)
C6F	-5170(20)	1344(19)	-4787(15)	33(5)
C7F	-5190(20)	-250(20)	-6222(14)	35(5)
C8F	-4940(20)	1410(20)	-3981(16)	31(6)
O71F	-4929(16)	-683(15)	-5807(11)	37(4)
O72F	-5410(20)	-492(19)	-6888(12)	61(6)
O81F	-4693(16)	856(14)	-3775(10)	35(4)
O82F	-5060(20)	1960(20)	-3606(14)	54(7)
N1G	-3238(17)	-543(16)	-4845(12)	32(4)
C2G	-3360(20)	-1388(19)	-4973(14)	22(5)
C3G	-2680(20)	-1560(20)	-5153(19)	43(7)
C4G	-1830(30)	-830(30)	-5200(20)	46(8)
C5G	-1660(30)	120(30)	-5020(20)	38(7)
C6G	-2400(20)	200(20)	-4849(15)	31(5)
C7G	-4300(20)	-2110(20)	-4895(15)	39(6)
C8G	-2390(20)	1100(20)	-4696(18)	28(6)
O71G	-4879(16)	-1843(14)	-4773(13)	42(4)
O72G	-4460(20)	-2931(17)	-4981(17)	57(7)
O81G	-3128(15)	1054(14)	-4595(12)	38(4)
O82G	-1624(19)	1831(18)	-4657(18)	54(7)
N1H	-5258(16)	-944(15)	-3529(11)	26(4)
C2H	-4685(19)	-756(18)	-2869(13)	27(5)
C3H	-5040(20)	-1040(20)	-2294(16)	39(7)
C4H	-6020(30)	-1530(30)	-2420(20)	59(9)
C5H	-6630(20)	-1750(20)	-3091(17)	47(7)
C6H	-6200(20)	-1413(19)	-3643(14)	33(5)
C7H	-3650(20)	-220(20)	-2841(14)	36(5)

C8H	-6730(20)	-1560(20)	-4396(17)	38(6)
O71H	-3450(15)	-2(16)	-3431(11)	30(4)
O72H	-3072(18)	-20(20)	-2262(13)	51(7)
O81H	-6225(14)	-1168(15)	-4805(10)	42(4)
O82H	-7612(16)	-2010(20)	-4559(14)	59(7)
N1I	-3992(17)	-1849(16)	162(12)	31(4)
C2I	-4320(20)	-1256(18)	157(15)	33(5)
C3I	-4080(30)	-570(20)	730(18)	43(7)
C4I	-3490(30)	-500(30)	1345(19)	42(9)
C5I	-3100(30)	-1110(20)	1360(17)	40(7)
C6I	-3390(20)	-1760(20)	739(15)	30(5)
C7I	-5010(20)	-1430(20)	-553(16)	43(6)
C8I	-3090(20)	-2470(20)	664(16)	28(6)
O71I	-5151(16)	-2101(15)	-1044(11)	41(5)
O72I	-5400(20)	-971(19)	-618(14)	54(6)
O81I	-3449(16)	-3021(15)	43(11)	41(4)
O82I	-2520(20)	-2480(20)	1168(14)	49(7)
N1J	-3084(16)	-3131(15)	-1383(11)	36(4)
C2J	-2292(19)	-2360(20)	-1402(15)	36(5)
C3J	-1530(20)	-2350(20)	-1579(18)	42(7)
C4J	-1610(30)	-3220(30)	-1780(20)	43(9)
C5J	-2420(20)	-4030(20)	-1772(19)	44(7)
C6J	-3160(20)	-3950(20)	-1575(15)	36(5)
C7J	-2330(20)	-1500(20)	-1175(15)	38(6)
C8J	-4080(20)	-4760(20)	-1524(17)	32(6)
O71J	-3083(15)	-1608(14)	-1005(12)	45(4)
O72J	-1641(19)	-738(17)	-1178(16)	54(7)
O81J	-4672(15)	-4582(14)	-1343(12)	37(4)
O82J	-4160(20)	-5568(17)	-1684(18)	53(7)
N1K	-6143(16)	-3952(15)	-1721(11)	37(4)
C2K	-6831(18)	-4413(18)	-1419(14)	37(5)
C3K	-7790(20)	-4850(20)	-1759(18)	43(7)
C4K	-8020(30)	-4720(30)	-2530(20)	58(8)
C5K	-7320(20)	-4250(30)	-2800(18)	57(7)
C6K	-6350(19)	-3858(19)	-2377(14)	38(5)
C7K	-6500(20)	-4440(20)	-639(15)	36(6)
C8K	-5500(20)	-3270(20)	-2646(16)	47(6)
O71K	-5631(15)	-3969(16)	-381(11)	45(4)
O72K	-7105(17)	-4880(20)	-344(13)	64(6)
O81K	-4693(14)	-2994(15)	-2197(11)	46(4)
O82K	-5587(19)	-3160(20)	-3242(13)	58(7)
N1L	-11304(16)	-4805(16)	108(12)	34(4)
C2L	-11300(20)	-3978(19)	180(14)	46(5)
C3L	-12040(20)	-3910(20)	333(19)	59(7)
C4L	-12880(30)	-4760(30)	320(20)	62(9)
C5L	-12900(20)	-5600(30)	260(20)	57(7)
C6L	-12090(20)	-5540(20)	139(15)	45(5)
C7L	-10360(20)	-3180(20)	165(16)	47(6)

C8L	-12000(20)	-6440(20)	-4(18)	46(7)
O71L	-9766(15)	-3425(14)	52(12)	49(4)
O72L	-10230(20)	-2436(16)	244(17)	81(7)
O81L	-11227(15)	-6288(14)	-138(12)	36(4)
O82L	-12710(20)	-7174(17)	-27(18)	71(7)
N1M	-9180(16)	-3977(14)	-1068(11)	34(4)
C2M	-9701(19)	-4089(18)	-1701(13)	27(5)
C3M	-9350(30)	-3570(20)	-2178(17)	40(7)
C4M	-8400(30)	-2900(30)	-1980(20)	50(9)
C5M	-7800(20)	-2750(20)	-1332(16)	51(7)
C6M	-8250(20)	-3316(19)	-882(14)	32(5)
C7M	-10730(20)	-4841(19)	-1816(14)	34(5)
C8M	-7690(20)	-3260(20)	-156(16)	50(6)
O71M	-10958(15)	-5156(15)	-1295(11)	45(5)
O72M	-11308(19)	-5050(20)	-2433(13)	60(7)
O81M	-8208(14)	-3825(14)	201(10)	44(4)
O82M	-6856(17)	-2690(20)	67(14)	80(7)
N1N	-9338(16)	-5857(15)	375(12)	27(4)
C2N	-9209(19)	-5813(19)	1095(14)	29(5)
C3N	-9120(30)	-6470(20)	1415(18)	44(7)
C4N	-9170(30)	-7190(30)	940(20)	59(9)
C5N	-9260(30)	-7240(20)	232(18)	46(7)
C6N	-9350(20)	-6556(19)	-46(14)	35(5)
C7N	-9190(20)	-5010(20)	1496(14)	33(5)
C8N	-9550(20)	-6510(20)	-833(16)	31(6)
O71N	-9460(17)	-4556(15)	1134(11)	45(4)
O72N	-8910(20)	-4762(19)	2170(12)	56(6)
O81N	-9703(16)	-5909(14)	-976(10)	33(4)
O82N	-9500(20)	-7094(19)	-1274(14)	59(7)
N1O	-10431(16)	-3284(15)	-4863(12)	30(4)
C2O	-10010(20)	-3766(19)	-4773(15)	32(5)
C3O	-10180(30)	-4470(20)	-5335(18)	55(7)
C4O	-10830(30)	-4660(30)	-5980(20)	44(9)
C5O	-11280(30)	-4150(20)	-6071(17)	43(7)
C6O	-11050(20)	-3446(19)	-5468(15)	34(5)
C7O	-9320(20)	-3483(19)	-4062(16)	36(5)
C8O	-11470(20)	-2830(20)	-5469(16)	38(6)
O71O	-9285(16)	-2835(16)	-3622(11)	37(4)
O72O	-8837(19)	-3849(19)	-3928(15)	53(6)
O81O	-11175(16)	-2232(15)	-4861(11)	43(4)
O82O	-12010(20)	-2880(20)	-6004(13)	53(7)
N1P	-8506(15)	-878(15)	-3032(11)	34(4)
C2P	-8316(19)	-783(18)	-2324(13)	36(5)
C3P	-7430(20)	-200(20)	-1877(17)	54(7)
C4P	-6700(20)	350(30)	-2240(20)	72(8)
C5P	-6880(20)	240(20)	-2950(17)	54(7)
C6P	-7830(19)	-408(19)	-3329(14)	43(5)
C7P	-9180(20)	-1370(20)	-2069(14)	41(5)

C8P	-8160(20)	-580(20)	-4139(16)	41(6)
O71P	-9923(15)	-1918(15)	-2538(10)	43(4)
O72P	-9066(19)	-1220(20)	-1395(12)	68(6)
O81P	-9044(14)	-1198(15)	-4411(10)	43(4)
O82P	-7593(19)	-100(20)	-4460(14)	66(7)
N1Q	-6111(15)	-7732(15)	-8658(12)	35(4)
C2Q	-6842(18)	-8314(18)	-8428(14)	35(5)
C3Q	-7700(20)	-8930(20)	-8833(18)	62(7)
C4Q	-7880(30)	-8970(30)	-9560(20)	72(9)
C5Q	-7130(20)	-8400(20)	-9855(17)	57(7)
C6Q	-6237(19)	-7766(19)	-9359(14)	43(5)
C7Q	-6560(20)	-8210(20)	-7621(16)	39(6)
C8Q	-5360(20)	-7080(20)	-9554(16)	45(6)
O71Q	-5746(15)	-7535(15)	-7296(11)	39(4)
O72Q	-7141(18)	-8733(19)	-7324(14)	58(7)
O81Q	-4620(14)	-6617(15)	-9040(11)	47(4)
O82Q	-5450(20)	-7050(20)	-10190(13)	77(7)
N1R	-11627(16)	-2157(16)	-3443(12)	35(4)
C2R	-11670(20)	-1376(19)	-3288(14)	43(5)
C3R	-12470(20)	-1390(20)	-3154(18)	51(7)
C4R	-13270(30)	-2260(30)	-3160(20)	57(9)
C5R	-13250(20)	-3090(20)	-3334(19)	46(7)
C6R	-12380(20)	-2970(20)	-3463(16)	36(5)
C7R	-10770(20)	-520(20)	-3276(15)	47(5)
C8R	-12220(20)	-3780(20)	-3613(17)	32(6)
O71R	-10145(15)	-631(14)	-3467(12)	43(4)
O72R	-10750(20)	205(17)	-3052(17)	68(7)
O81R	-11403(15)	-3561(14)	-3742(12)	42(4)
O82R	-12870(20)	-4570(17)	-3627(18)	57(7)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Ce-I. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	21.9(4)	24.8(4)	27.3(4)	3.9(3)	7.3(3)	13.7(3)
Ce1	25.0(6)	33.7(7)	31.0(6)	10.7(5)	6.8(5)	19.2(6)
O11W	60(17)	90(20)	70(20)	23(18)	32(17)	41(16)
O12W	21(9)	70(13)	34(9)	7(9)	-2(7)	-1(9)
O13W	43(13)	100(19)	63(15)	52(15)	19(11)	33(13)
O14W	57(15)	120(20)	100(30)	30(20)	17(16)	65(17)
O15W	39(12)	54(15)	45(10)	8(10)	8(8)	6(11)
O16W	80(20)	64(16)	93(18)	27(14)	46(16)	43(16)
O17W	60(20)	80(20)	47(13)	-8(13)	0(13)	30(18)
O18W	29(11)	55(13)	85(19)	7(12)	4(11)	22(10)
U6	32.1(5)	27.1(4)	28.5(4)	5.3(3)	11.0(3)	17.7(4)
U3	24.2(4)	26.7(4)	22.8(4)	7.1(3)	8.8(3)	14.9(4)
U2	25.1(4)	26.0(4)	25.3(4)	6.2(3)	7.8(3)	16.1(4)

Ce4	31.2(7)	28.3(7)	30.2(7)	4.8(5)	6.1(5)	9.9(6)
U5	23.9(4)	25.8(4)	24.7(4)	7.3(3)	7.2(3)	13.7(4)
O41W	60(13)	37(10)	44(13)	0(9)	0(10)	20(10)
O42W	39(11)	52(16)	58(16)	4(13)	18(10)	18(11)
O43W	33(10)	75(14)	30(9)	15(9)	7(7)	28(10)
O44W	47(13)	56(15)	65(15)	15(12)	23(11)	22(12)
O45W	73(17)	61(15)	70(17)	35(13)	42(15)	39(14)
O46W	53(14)	43(14)	53(13)	10(10)	14(10)	24(12)
O47W	70(20)	80(20)	120(30)	40(20)	40(20)	40(20)
Ce3	31.2(7)	28.1(7)	30.1(6)	2.6(5)	9.2(5)	15.6(6)
U4	31.2(5)	30.3(5)	25.4(4)	1.8(3)	10.4(3)	15.6(4)
O31W	33(17)	90(20)	77(16)	0(15)	12(13)	37(18)
O32W	67(17)	62(16)	85(17)	57(14)	34(13)	44(14)
O33W	81(16)	70(16)	36(11)	16(11)	35(11)	27(13)
O34W	34(15)	110(30)	63(18)	40(19)	-3(13)	-3(17)
O35W	66(18)	51(14)	42(12)	13(11)	13(12)	43(14)
O36W	31(12)	68(16)	61(11)	-2(10)	21(9)	15(11)
Ce2	24.8(6)	29.3(7)	35.3(7)	8.2(5)	3.1(5)	16.0(5)
O21W	51(15)	70(20)	110(20)	18(17)	19(15)	47(16)
O22W	61(15)	70(16)	64(18)	38(14)	34(13)	41(14)
O23W	59(14)	38(13)	57(17)	11(11)	22(12)	8(11)
O24W	47(13)	42(11)	60(14)	27(10)	0(11)	18(10)
O25W	55(15)	100(20)	31(9)	15(11)	10(9)	55(16)
O26W	26(11)	36(14)	110(20)	-6(14)	0(13)	15(11)
O27W	43(12)	35(11)	93(19)	-10(11)	5(12)	18(10)
O28W	110(20)	70(20)	50(20)	-6(16)	10(17)	52(19)
N1A	44(11)	30(11)	33(10)	4(8)	15(8)	22(9)
C2A	45(13)	40(13)	31(12)	8(10)	10(10)	32(11)
C3A	51(17)	41(17)	70(17)	16(14)	26(14)	31(15)
C4A	42(19)	60(20)	70(20)	15(18)	30(16)	33(19)
C5A	28(16)	32(18)	53(19)	10(15)	19(14)	21(15)
C6A	26(14)	37(13)	43(13)	8(10)	15(11)	24(12)
C7A	46(15)	29(13)	55(12)	3(10)	22(11)	20(12)
C8A	31(16)	26(14)	37(15)	5(12)	-3(12)	16(12)
O71A	35(10)	28(10)	59(12)	-3(9)	15(9)	10(9)
O72A	78(17)	28(12)	108(19)	27(12)	46(14)	32(12)
O81A	33(10)	33(10)	47(12)	16(9)	19(9)	21(8)
O82A	23(13)	38(12)	80(20)	15(13)	12(13)	8(11)
N1B	27(11)	27(11)	47(10)	9(8)	15(8)	18(9)
C2B	14(13)	23(12)	42(13)	2(10)	6(10)	10(11)
C3B	63(18)	53(16)	42(15)	6(12)	6(13)	43(15)
C4B	60(20)	60(20)	19(16)	-3(14)	-12(15)	37(18)
C5B	39(19)	41(16)	27(14)	2(12)	-15(13)	27(15)
C6B	35(14)	35(13)	36(12)	7(10)	7(10)	19(11)
C7B	32(14)	32(14)	38(14)	16(11)	20(11)	21(12)
C8B	41(15)	45(15)	39(15)	19(12)	25(12)	37(13)
O71B	28(12)	28(11)	31(10)	9(8)	14(8)	7(10)
O72B	22(19)	43(15)	47(14)	9(12)	4(13)	20(15)

O81B	62(12)	50(11)	33(9)	4(8)	3(8)	46(10)
O82B	88(18)	82(17)	40(12)	11(12)	0(12)	78(15)
N1C	21(10)	28(11)	18(10)	-2(8)	-2(8)	12(9)
C2C	33(13)	48(12)	28(11)	4(9)	15(9)	21(11)
C3C	24(15)	59(17)	42(15)	8(13)	3(12)	24(13)
C4C	52(16)	50(20)	50(20)	5(16)	16(14)	14(15)
C5C	31(14)	63(17)	36(15)	14(12)	10(11)	10(13)
C6C	43(13)	38(13)	27(12)	24(10)	12(9)	19(11)
C7C	18(14)	29(14)	43(12)	10(10)	12(10)	5(12)
C8C	46(16)	52(15)	52(13)	25(12)	31(12)	34(13)
O71C	27(10)	40(11)	31(9)	4(8)	9(8)	10(9)
O72C	49(14)	75(19)	27(10)	6(11)	12(9)	35(13)
O81C	35(9)	39(11)	31(9)	15(8)	7(7)	20(8)
O82C	49(13)	95(17)	54(13)	40(12)	22(10)	23(12)
N1D	21(11)	33(11)	32(10)	7(8)	10(8)	17(9)
C2D	29(12)	17(13)	27(12)	6(10)	6(9)	13(11)
C3D	40(16)	49(18)	59(18)	11(14)	23(13)	15(14)
C4D	50(20)	70(20)	80(20)	32(17)	36(16)	47(19)
C5D	49(15)	48(18)	71(18)	13(14)	18(13)	34(14)
C6D	24(13)	32(13)	55(12)	6(10)	16(10)	10(11)
C7D	27(14)	35(13)	30(12)	3(10)	7(10)	17(11)
C8D	36(16)	33(13)	65(15)	1(11)	23(12)	21(12)
O71D	39(10)	25(10)	47(12)	4(9)	16(9)	22(8)
O72D	40(12)	26(12)	55(18)	1(11)	20(12)	11(10)
O81D	37(10)	27(10)	74(12)	17(8)	27(9)	17(8)
O82D	54(15)	34(11)	130(20)	7(12)	30(14)	32(11)
N1E	27(10)	35(10)	25(10)	8(8)	11(8)	16(9)
C2E	26(12)	35(12)	42(13)	11(10)	9(10)	15(10)
C3E	52(18)	38(16)	35(15)	-5(12)	17(13)	28(15)
C4E	80(20)	55(19)	43(17)	5(14)	15(15)	40(17)
C5E	72(18)	38(17)	43(14)	2(12)	20(13)	31(15)
C6E	36(13)	29(13)	26(13)	-5(10)	1(10)	21(11)
C7E	45(13)	22(13)	43(15)	12(11)	15(11)	25(11)
C8E	38(14)	41(16)	38(14)	9(12)	14(11)	14(13)
O71E	40(11)	45(11)	29(10)	7(8)	6(8)	28(10)
O72E	72(16)	42(15)	60(14)	13(12)	18(12)	47(14)
O81E	51(12)	34(11)	24(9)	-4(8)	0(8)	30(10)
O82E	75(19)	63(18)	16(12)	10(12)	-10(12)	44(16)
N1F	12(11)	29(10)	24(10)	7(8)	-2(8)	10(9)
C2F	23(12)	38(13)	23(12)	2(9)	9(9)	13(10)
C3F	58(18)	45(17)	44(15)	6(13)	1(13)	26(15)
C4F	80(20)	61(19)	40(20)	34(16)	9(17)	53(18)
C5F	56(18)	30(17)	51(15)	-1(13)	-2(13)	24(15)
C6F	38(13)	46(13)	28(12)	10(10)	10(10)	28(11)
C7F	19(13)	56(13)	28(12)	8(10)	3(10)	19(11)
C8F	41(15)	37(15)	21(14)	10(11)	12(11)	23(13)
O71F	51(12)	37(11)	23(9)	4(8)	8(8)	25(10)
O72F	106(19)	52(14)	28(10)	9(9)	15(10)	43(14)

O81F	55(12)	44(11)	23(9)	10(8)	16(8)	36(10)
O82F	90(20)	50(16)	38(13)	7(11)	22(13)	47(16)
N1G	47(11)	30(11)	28(10)	6(8)	21(8)	25(9)
C2G	30(13)	24(12)	27(12)	6(9)	18(10)	21(11)
C3G	54(17)	42(17)	60(17)	14(13)	29(13)	39(15)
C4G	39(19)	50(20)	70(20)	7(17)	13(16)	43(18)
C5G	35(17)	61(18)	40(19)	24(15)	37(14)	31(15)
C6G	31(14)	38(13)	37(13)	10(10)	15(10)	25(11)
C7G	54(15)	35(13)	37(12)	13(10)	20(11)	27(12)
C8G	30(15)	27(14)	31(15)	7(11)	16(12)	15(12)
O71G	34(10)	43(10)	60(12)	10(9)	23(9)	25(8)
O72G	88(16)	23(11)	82(18)	21(11)	52(14)	33(12)
O81G	34(10)	33(10)	49(12)	14(8)	15(9)	17(8)
O82G	29(13)	37(12)	90(20)	15(12)	23(13)	13(11)
N1H	24(10)	30(10)	33(9)	16(8)	14(8)	16(9)
C2H	17(13)	29(12)	33(11)	6(9)	4(9)	12(11)
C3H	24(17)	53(18)	40(14)	15(13)	11(12)	18(15)
C4H	50(20)	80(20)	45(18)	28(16)	28(16)	27(18)
C5H	43(17)	60(18)	33(14)	21(13)	15(13)	17(15)
C6H	33(13)	37(13)	29(12)	4(10)	6(10)	20(11)
C7H	33(14)	51(14)	18(11)	-1(10)	-2(10)	21(12)
C8H	29(13)	64(15)	15(15)	8(12)	0(11)	21(12)
O71H	22(10)	26(12)	33(10)	10(9)	3(8)	5(9)
O72H	34(13)	86(19)	32(11)	17(12)	9(9)	28(13)
O81H	28(9)	54(11)	27(9)	7(8)	1(7)	11(9)
O82H	22(11)	82(17)	47(14)	26(12)	7(10)	4(11)
N1I	33(11)	32(11)	36(10)	8(8)	11(8)	22(9)
C2I	47(13)	25(12)	39(13)	11(10)	27(10)	22(11)
C3I	72(19)	33(16)	45(15)	19(12)	27(13)	37(15)
C4I	50(20)	45(19)	30(16)	2(14)	7(15)	21(17)
C5I	49(19)	43(15)	31(15)	9(12)	5(13)	29(14)
C6I	15(14)	37(13)	38(12)	11(10)	15(10)	9(11)
C7I	37(14)	46(14)	53(14)	24(11)	16(11)	23(12)
C8I	35(15)	26(15)	33(14)	13(12)	24(11)	17(13)
O71I	46(12)	38(10)	36(10)	3(8)	8(8)	21(9)
O72I	69(18)	62(15)	53(14)	12(11)	11(12)	52(15)
O81I	51(11)	41(11)	38(9)	1(8)	5(8)	33(10)
O82I	52(16)	53(16)	47(13)	11(11)	5(11)	34(14)
N1J	45(11)	38(10)	26(10)	3(8)	12(8)	21(9)
C2J	40(12)	38(13)	30(12)	6(10)	9(9)	20(10)
C3J	46(15)	16(18)	61(17)	-1(14)	20(13)	16(14)
C4J	43(19)	60(20)	40(20)	11(18)	17(16)	29(19)
C5J	23(14)	52(17)	57(18)	4(14)	23(13)	17(13)
C6J	41(13)	37(13)	34(12)	7(10)	15(10)	23(11)
C7J	30(13)	28(13)	53(12)	12(10)	16(10)	11(11)
C8J	26(15)	31(13)	34(15)	9(11)	8(12)	10(12)
O71J	51(10)	38(9)	47(12)	14(8)	17(9)	21(8)
O72J	41(13)	34(11)	68(18)	5(11)	18(12)	4(10)

O81J	34(10)	29(9)	36(12)	0(8)	9(9)	9(8)
O82J	51(16)	33(12)	80(20)	0(12)	31(14)	21(11)
N1K	39(10)	35(10)	36(9)	6(8)	10(8)	19(8)
C2K	30(12)	45(12)	37(12)	3(10)	5(9)	22(10)
C3K	30(14)	48(17)	46(16)	5(13)	4(12)	19(13)
C4K	29(16)	70(20)	57(19)	-3(15)	2(14)	19(15)
C5K	46(14)	66(18)	54(16)	13(13)	8(11)	27(13)
C6K	33(12)	39(13)	41(12)	7(10)	11(9)	18(10)
C7K	42(13)	38(12)	33(13)	11(10)	16(10)	21(11)
C8K	53(16)	45(16)	41(13)	6(11)	14(11)	24(13)
O71K	41(10)	67(12)	36(9)	21(8)	22(8)	28(9)
O72K	44(12)	73(16)	45(12)	12(11)	21(10)	5(12)
O81K	43(9)	57(11)	25(9)	6(8)	4(7)	19(8)
O82K	48(15)	90(19)	42(12)	30(12)	13(10)	36(14)
N1L	25(10)	40(10)	36(10)	11(8)	7(8)	18(9)
C2L	58(13)	62(12)	44(11)	17(9)	20(9)	46(11)
C3L	52(16)	94(17)	56(17)	22(14)	6(13)	59(14)
C4L	59(18)	100(20)	50(20)	24(17)	19(15)	58(18)
C5L	38(16)	83(18)	59(18)	22(14)	18(14)	35(15)
C6L	48(13)	50(13)	39(13)	8(10)	12(10)	27(11)
C7L	58(14)	51(13)	43(13)	12(10)	11(11)	36(12)
C8L	41(16)	44(13)	41(15)	3(11)	22(12)	11(12)
O71L	47(11)	38(10)	66(12)	13(8)	19(9)	24(9)
O72L	89(14)	45(11)	122(19)	8(11)	39(13)	43(11)
O81L	34(10)	33(10)	40(12)	7(9)	13(9)	16(8)
O82L	49(14)	51(12)	100(20)	10(12)	35(14)	8(11)
N1M	37(11)	42(10)	39(9)	21(8)	15(8)	28(9)
C2M	32(13)	28(12)	26(10)	9(9)	9(9)	19(11)
C3M	42(18)	44(17)	41(14)	27(13)	18(13)	21(15)
C4M	40(20)	70(19)	34(19)	36(16)	20(17)	19(17)
C5M	44(17)	69(17)	40(14)	28(12)	9(12)	26(14)
C6M	10(13)	38(12)	34(12)	10(10)	4(10)	3(11)
C7M	23(14)	28(13)	39(12)	10(10)	3(10)	4(11)
C8M	33(13)	52(14)	48(14)	13(11)	-2(10)	12(11)
O71M	29(10)	64(11)	26(9)	11(8)	-4(7)	16(9)
O72M	57(14)	82(15)	24(11)	14(10)	-4(10)	26(12)
O81M	19(9)	57(11)	43(9)	25(8)	9(7)	7(8)
O82M	27(11)	78(16)	76(14)	41(12)	-4(10)	-16(11)
N1N	19(11)	35(10)	27(10)	9(8)	9(8)	13(9)
C2N	21(12)	41(12)	19(11)	9(9)	-1(9)	13(10)
C3N	58(18)	54(16)	31(16)	18(13)	13(13)	36(15)
C4N	60(20)	65(18)	70(20)	34(16)	11(17)	38(18)
C5N	72(18)	39(16)	35(16)	23(13)	15(13)	32(15)
C6N	38(14)	38(13)	32(12)	9(10)	8(10)	23(11)
C7N	22(13)	48(13)	29(12)	15(10)	14(10)	13(11)
C8N	32(15)	16(15)	38(14)	-6(11)	3(11)	10(13)
O71N	65(12)	47(11)	33(9)	7(8)	14(8)	35(10)
O72N	86(19)	71(14)	31(10)	8(9)	13(10)	57(14)

O81N	26(12)	41(10)	29(9)	3(8)	3(8)	18(10)
O82N	100(20)	52(15)	33(12)	9(11)	23(12)	49(15)
N1O	25(10)	27(10)	37(10)	6(8)	9(8)	13(9)
C2O	34(12)	40(12)	33(12)	17(10)	15(10)	24(10)
C3O	56(18)	59(16)	69(16)	11(12)	23(13)	43(14)
C4O	70(20)	30(18)	45(18)	16(14)	32(15)	29(17)
C5O	46(18)	31(16)	47(15)	-1(12)	10(13)	19(15)
C6O	37(13)	36(13)	31(13)	8(10)	13(10)	19(11)
C7O	32(13)	32(13)	55(14)	20(11)	14(11)	20(11)
C8O	41(14)	33(16)	47(14)	17(12)	13(11)	23(12)
O71O	42(11)	47(11)	35(10)	15(8)	13(8)	31(10)
O72O	64(14)	59(15)	57(15)	10(12)	7(12)	52(13)
O81O	65(11)	51(10)	24(9)	7(8)	6(8)	40(9)
O82O	57(16)	67(18)	41(12)	6(11)	-8(11)	46(15)
N1P	37(10)	31(11)	27(10)	1(8)	7(8)	13(9)
C2P	40(12)	25(12)	37(11)	8(9)	6(9)	14(10)
C3P	35(15)	58(17)	46(14)	-5(12)	1(11)	13(13)
C4P	37(16)	84(19)	60(20)	12(15)	-4(14)	8(15)
C5P	31(15)	65(16)	36(15)	8(12)	-2(11)	6(13)
C6P	31(13)	51(13)	35(12)	4(10)	8(9)	15(11)
C7P	31(14)	55(14)	29(12)	3(10)	1(10)	20(12)
C8P	40(16)	34(15)	41(13)	5(11)	22(12)	9(13)
O71P	37(10)	35(11)	46(9)	12(8)	18(7)	7(9)
O72P	49(14)	103(17)	39(10)	22(10)	21(9)	25(13)
O81P	30(9)	37(10)	48(9)	9(8)	15(7)	5(8)
O82P	68(14)	64(16)	42(13)	8(11)	25(11)	13(12)
N1Q	35(10)	37(10)	34(10)	7(8)	5(8)	22(9)
C2Q	16(12)	34(11)	42(12)	10(10)	7(10)	4(10)
C3Q	42(14)	56(16)	59(16)	11(13)	2(12)	8(13)
C4Q	49(17)	75(19)	68(19)	25(15)	5(14)	14(15)
C5Q	40(14)	58(15)	43(15)	5(12)	-2(12)	8(12)
C6Q	35(12)	50(13)	32(12)	6(10)	1(10)	16(11)
C7Q	39(13)	43(14)	40(14)	19(11)	13(11)	22(11)
C8Q	38(16)	52(15)	31(13)	14(12)	5(12)	13(13)
O71Q	46(10)	44(10)	35(9)	9(8)	12(8)	30(9)
O72Q	38(13)	58(15)	68(14)	34(12)	23(10)	10(11)
O81Q	41(9)	59(10)	22(9)	11(8)	11(7)	11(8)
O82Q	71(15)	105(16)	45(11)	25(11)	29(10)	32(13)
N1R	34(10)	44(10)	33(10)	6(8)	8(8)	25(9)
C2R	51(13)	53(12)	35(11)	13(9)	5(9)	36(11)
C3R	35(16)	65(18)	52(17)	16(14)	17(13)	21(15)
C4R	41(17)	80(20)	70(20)	26(17)	19(15)	44(17)
C5R	44(16)	61(18)	51(17)	31(14)	26(13)	33(14)
C6R	42(13)	41(13)	35(13)	9(10)	13(10)	28(11)
C7R	51(14)	38(13)	48(12)	6(10)	7(10)	22(11)
C8R	45(15)	38(13)	19(14)	9(11)	7(12)	25(12)
O71R	38(10)	35(9)	66(11)	11(8)	23(9)	23(8)
O72R	88(15)	45(11)	77(19)	-9(11)	18(13)	45(11)

O81R	39(10)	41(9)	49(12)	12(8)	20(9)	21(8)
O82R	51(14)	53(11)	40(20)	2(12)	12(14)	11(10)

Table 4 Bond Lengths for U-Ce-I.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	N1A	2.54(2)		C3F	C4F	1.41(5)
U1	O71A	2.37(2)		C4F	C5F	1.44(5)
U1	O81A	2.46(2)		C5F	C6F	1.38(4)
U1	N1B	2.56(2)		C6F	C8F	1.53(4)
U1	O71B	2.45(2)		C7F	O71F	1.30(4)
U1	O81B	2.36(2)		C7F	O72F	1.25(3)
U1	N1Q	2.50(2)		C8F	O81F	1.26(4)
U1	O71Q	2.36(2)		C8F	O82F	1.24(4)
U1	O81Q	2.41(2)		O82F	$Ce3^4$	2.44(3)
Ce1	O11W	2.61(3)		N1G	C2G	1.33(4)
Ce1	O12W	2.531(19)		N1G	C6G	1.36(4)
Ce1	O13W	2.51(2)		C2G	C3G	1.37(4)
Ce1	O14W	2.60(3)		C2G	C7G	1.50(4)
Ce1	O15W	2.56(2)		C3G	C4G	1.38(5)
Ce1	O16W	2.61(3)		C4G	C5G	1.46(5)
Ce1	O17W	2.58(3)		C5G	C6G	1.39(4)
Ce1	O18W	2.52(2)		C6G	C8G	1.49(4)
Ce1	O72B	2.43(2)		C7G	O71G	1.28(4)
U6	N1O	2.54(2)		C7G	O72G	1.26(4)
U6	O71O	2.34(2)		C8G	O81G	1.24(4)
U6	O81O	2.33(2)		C8G	O82G	1.26(4)
U6	N1P	2.53(2)		N1H	C2H	1.36(3)
U6	O71P	2.358(19)		N1H	C6H	1.33(4)
U6	O81P	2.40(2)		C2H	C3H	1.39(4)
U6	N1R	2.56(2)		C2H	C7H	1.48(4)
U6	O71R	2.45(2)		C3H	C4H	1.37(5)
U6	O81R	2.36(2)		C4H	C5H	1.38(5)
U3	N1F	2.55(2)		C5H	C6H	1.41(4)
U3	O71F	2.39(2)		C6H	C8H	1.50(4)
U3	O81F	2.45(2)		C7H	O71H	1.30(3)
U3	N1G	2.53(2)		C7H	O72H	1.23(3)
U3	O71G	2.34(2)		C8H	O81H	1.26(4)
U3	O81G	2.41(2)		C8H	O82H	1.23(4)
U3	N1H	2.54(2)		N1I	C2I	1.35(4)
U3	O71H	2.36(2)		N1I	C6I	1.30(4)
U3	O81H	2.35(2)		C2I	C3I	1.36(4)
U2	N1C	2.54(2)		C2I	C7I	1.52(4)
U2	O71C	2.42(2)		C3I	C4I	1.36(5)
U2	O81C	2.36(2)		C4I	C5I	1.44(5)
U2	N1D	2.53(2)		C5I	C6I	1.37(4)
U2	O71D	2.43(2)		C6I	C8I	1.52(4)

U2	O81D	2.34(2)		C7I	O71I	1.29(4)
U2	N1E	2.52(2)		C7I	O72I	1.23(4)
U2	O71E	2.40(2)		C8I	O81I	1.27(4)
U2	O81E	2.34(2)		C8I	O82I	1.24(4)
Ce4	O41W	2.55(2)		N1J	C2J	1.34(3)
Ce4	O42W	2.55(3)		N1J	C6J	1.33(4)
Ce4	O43W	2.514(19)		C2J	C3J	1.36(4)
Ce4	O44W	2.47(3)		C2J	C7J	1.50(4)
Ce4	O45W	2.56(2)		C3J	C4J	1.41(6)
Ce4	O46W	2.57(2)		C4J	C5J	1.38(5)
Ce4	O47W	2.64(4)		C5J	C6J	1.40(4)
Ce4	O82N	2.51(2)		C6J	C8J	1.52(4)
Ce4	O72R[1]	2.49(2)		C7J	O71J	1.28(4)
U5	N1L	2.51(2)		C7J	O72J	1.25(4)
U5	O71L	2.30(2)		C8J	O81J	1.25(4)
U5	O81L	2.38(2)		C8J	O82J	1.30(4)
U5	N1M	2.53(2)		N1K	C2K	1.32(3)
U5	O71M	2.40(2)		N1K	C6K	1.31(3)
U5	O81M	2.369(19)		C2K	C3K	1.38(4)
U5	N1N	2.52(2)		C2K	C7K	1.54(4)
U5	O71N	2.41(2)		C3K	C4K	1.55(5)
U5	O81N	2.42(2)		C4K	C5K	1.30(5)
Ce3	O31W	2.44(3)		C5K	C6K	1.44(4)
Ce3	O32W	2.58(2)		C6K	C8K	1.51(4)
Ce3	O33W	2.54(2)		C7K	O71K	1.22(4)
Ce3	O34W	2.44(3)		C7K	O72K	1.22(4)
Ce3	O35W	2.53(2)		C8K	O81K	1.28(4)
Ce3	O36W	2.48(2)		C8K	O82K	1.19(4)
Ce3	O82F[1]	2.44(3)		N1L	C2L	1.38(4)
Ce3	O82J	2.42(3)		N1L	C6L	1.31(4)
U4	N1I	2.52(2)		C2L	C3L	1.36(4)
U4	O71I	2.37(2)		C2L	C7L	1.50(4)
U4	O81I	2.33(2)		C3L	C4L	1.45(5)
U4	N1J	2.55(2)		C4L	C5L	1.40(5)
U4	O71J	2.35(2)		C5L	C6L	1.37(4)
U4	O81J	2.47(2)		C6L	C8L	1.59(4)
U4	N1K	2.53(2)		C7L	O71L	1.27(4)
U4	O71K	2.48(2)		C7L	O72L	1.15(4)
U4	O81K	2.348(19)		C8L	O81L	1.26(4)
Ce2	O21W	2.56(3)		C8L	O82L	1.21(4)
Ce2	O22W	2.61(3)		N1M	C2M	1.31(3)
Ce2	O23W	2.44(3)		N1M	C6M	1.34(3)
Ce2	O24W	2.48(2)		C2M	C3M	1.37(4)
Ce2	O25W	2.58(2)		C2M	C7M	1.51(4)
Ce2	O26W	2.52(2)		C3M	C4M	1.37(5)
Ce2	O27W	2.57(2)		C4M	C5M	1.37(5)
Ce2	O28W	2.50(3)		C5M	C6M	1.41(4)
Ce2	O72E[2]	2.42(2)		C6M	C8M	1.51(4)

N1A	C2A	1.33(4)		C7M	O71M	1.23(3)
N1A	C6A	1.34(4)		C7M	O72M	1.28(3)
C2A	C3A	1.39(4)		C8M	O81M	1.31(4)
C2A	C7A	1.50(4)		C8M	O82M	1.19(4)
C3A	C4A	1.34(6)		N1N	C2N	1.37(3)
C4A	C5A	1.43(6)		N1N	C6N	1.34(4)
C5A	C6A	1.35(4)		C2N	C3N	1.39(4)
C6A	C8A	1.54(4)		C2N	C7N	1.47(4)
C7A	O71A	1.23(4)		C3N	C4N	1.40(5)
C7A	O72A	1.27(4)		C4N	C5N	1.34(5)
C8A	O81A	1.24(4)		C5N	C6N	1.40(4)
C8A	O82A	1.22(4)		C6N	C8N	1.53(4)
N1B	C2B	1.38(4)		C7N	O71N	1.28(4)
N1B	C6B	1.32(4)		C7N	O72N	1.26(3)
C2B	C3B	1.38(4)		C8N	O81N	1.21(4)
C2B	C7B	1.52(4)		C8N	O82N	1.27(4)
C3B	C4B	1.46(5)		N1O	C2O	1.31(4)
C4B	C5B	1.43(5)		N1O	C6O	1.31(4)
C5B	C6B	1.41(4)		C2O	C3O	1.40(4)
C6B	C8B	1.45(4)		C2O	C7O	1.48(4)
C7B	O71B	1.26(4)		C3O	C4O	1.40(5)
C7B	O72B	1.24(4)		C4O	C5O	1.39(6)
C8B	O81B	1.25(4)		C5O	C6O	1.41(4)
C8B	O82B	1.28(4)		C6O	C8O	1.50(4)
N1C	C2C	1.30(3)		C7O	O71O	1.28(4)
N1C	C6C	1.36(3)		C7O	O72O	1.23(4)
C2C	C3C	1.40(4)		C8O	O81O	1.31(4)
C2C	C7C	1.50(4)		C8O	O82O	1.22(4)
C3C	C4C	1.38(5)		N1P	C2P	1.33(3)
C4C	C5C	1.45(5)		N1P	C6P	1.30(3)
C5C	C6C	1.31(4)		C2P	C3P	1.36(4)
C6C	C8C	1.48(4)		C2P	C7P	1.51(4)
C7C	O71C	1.26(4)		C3P	C4P	1.48(5)
C7C	O72C	1.28(3)		C4P	C5P	1.33(5)
C8C	O81C	1.30(4)		C5P	C6P	1.40(4)
C8C	O82C	1.20(4)		C6P	C8P	1.52(4)
N1D	C2D	1.31(4)		C7P	O71P	1.23(3)
N1D	C6D	1.33(4)		C7P	O72P	1.27(3)
C2D	C3D	1.41(4)		C8P	O81P	1.28(4)
C2D	C7D	1.51(4)		C8P	O82P	1.24(4)
C3D	C4D	1.41(6)		N1Q	C2Q	1.34(3)
C4D	C5D	1.38(5)		N1Q	C6Q	1.34(3)
C5D	C6D	1.37(4)		C2Q	C3Q	1.31(4)
C6D	C8D	1.51(4)		C2Q	C7Q	1.52(4)
C7D	O71D	1.27(4)		C3Q	C4Q	1.37(5)
C7D	O72D	1.23(4)		C4Q	C5Q	1.43(5)
C8D	O81D	1.25(4)		C5Q	C6Q	1.42(4)
C8D	O82D	1.20(4)		C6Q	C8Q	1.50(4)

N1E	C2E	1.34(4)		C7Q	O71Q	1.25(4)
N1E	C6E	1.33(4)		C7Q	O72Q	1.24(4)
C2E	C3E	1.41(4)		C8Q	O81Q	1.26(4)
C2E	C7E	1.46(4)		C8Q	O82Q	1.23(4)
C3E	C4E	1.37(5)		N1R	C2R	1.36(3)
C4E	C5E	1.40(5)		N1R	C6R	1.33(4)
C5E	C6E	1.37(4)		C2R	C3R	1.38(4)
C6E	C8E	1.56(4)		C2R	C7R	1.50(4)
C7E	O71E	1.26(4)		C3R	C4R	1.42(5)
C7E	O72E	1.26(4)		C4R	C5R	1.41(5)
C8E	O81E	1.29(4)		C5R	C6R	1.42(4)
C8E	O82E	1.23(4)		C6R	C8R	1.53(4)
O72E	Ce2[3]	2.42(2)		C7R	O71R	1.24(4)
N1F	C2F	1.30(3)		C7R	O72R	1.24(4)
N1F	C6F	1.39(4)		C8R	O81R	1.29(4)
C2F	C3F	1.37(4)		C8R	O82R	1.24(4)
C2F	C7F	1.48(4)		O72R	Ce4[4]	2.49(2)

[1]+X,-1+Y,+Z; [2]-1+X,1+Y,+Z; [3]1+X,-1+Y,+Z; [4]+X,1+Y,+Z

II.14 U-La-II

Table 1 Crystal data and structure refinement for U-La-II.	
Identification code	U-La-II
Empirical formula	$C_{28}H_{20}LaN_4O_{26}U$
Formula weight	1205.42
Temperature/K	300.33
Crystal system	triclinic
Space group	P-1
a/Å	12.8597(5)
b/Å	13.0375(5)
c/Å	13.2067(5)
α/°	98.309(2)
β/°	119.231(2)
γ/°	90.328(2)
Volume/Å^3	1904.49(13)
Z	2
ρ_{calc}g/cm^3	2.102
μ/mm^{-1}	5.456
F(000)	1146.0
Crystal size/mm^3	0.166 × 0.114 × 0.07
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.17 to 61.56
Index ranges	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -18 ≤ l ≤ 18
Reflections collected	67639

Independent reflections	11616 [R_{int} = 0.0402, R_{sigma} = 0.0310]
Data/restraints/parameters	11616/0/545
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0266, wR_2 = 0.0647
Final R indexes [all data]	R_1 = 0.0334, wR_2 = 0.0680
Largest diff. peak/hole / e $Å^{-3}$	2.44/-1.50

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for U-La-II. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	7178.1(2)	7601.9(2)	2291.7(2)	20.78(3)
La1	8079.1(2)	6962.2(2)	7530.2(2)	23.89(4)
O71A	7576(2)	7009.4(19)	741.8(19)	29.4(5)
O71D	9570(2)	5682(2)	8343(2)	38.9(6)
O81A	5601(2)	8643.3(19)	2167(2)	32.6(5)
O72C	7323(3)	7906(2)	5817(2)	42.7(6)
O71C	7127(2)	7360.3(19)	4051(2)	33.5(5)
O71B	5485(2)	6414.7(18)	1440(2)	30.6(5)
O81D	5853(2)	6481.5(19)	6376(2)	32.4(5)
O72B	4532(2)	4824(2)	972(2)	39.2(6)
O72A	7362(2)	6952(2)	-1034(2)	37.7(6)
N1A	5756(2)	8064(2)	287(2)	22.4(5)
O82B	10694(2)	6207(2)	4052(3)	49.0(7)
O81C	8092(2)	9102(2)	2076(2)	38.9(6)
O81B	9210(2)	7253(2)	3391(2)	34.7(5)
O1W	8019(3)	5763(2)	5727(2)	42.8(6)
O82A	3716(2)	9022(2)	1132(2)	44.3(7)
N1D	7299(2)	5049(2)	7355(2)	26.8(5)
O72D	10172(3)	4166(2)	8913(3)	53.6(8)
N1C	8020(2)	9130(2)	4002(2)	24.3(5)
O2W	9941(2)	7609(2)	7522(3)	54.1(8)
N1B	7569(2)	5740(2)	2522(2)	23.4(5)
O4W	9767(3)	7581(3)	9820(3)	71.6(11)
O82D	4241(2)	5466(2)	5917(3)	48.0(7)
C6B	8688(3)	5467(3)	3114(3)	28.8(6)
O3S	3814(4)	9835(3)	3237(3)	67.3(10)
O2S	7760(3)	4634(3)	199(3)	54.8(8)
O82C	8923(3)	10723(3)	2603(3)	61.0(9)
O3W	7848(4)	8874(2)	8127(3)	63.7(10)
C7A	7058(3)	7215(2)	-294(3)	24.7(6)
O6S	11842(3)	7388(3)	9687(3)	56.1(8)
C6A	4800(3)	8559(2)	129(3)	26.0(6)
C2A	5983(3)	7833(2)	-602(3)	24.1(6)
C8A	4673(3)	8761(3)	1219(3)	29.0(7)
C3A	5266(3)	8127(3)	-1688(3)	30.7(7)
C7C	7419(3)	8041(3)	4953(3)	28.3(6)
C2C	7927(3)	9074(3)	4957(3)	27.7(6)
C4A	4272(3)	8653(3)	-1846(3)	36.5(8)

O1S	6944(3)	2856(3)	4617(3)	67.7(10)
C7B	5444(3)	5430(3)	1429(3)	27.7(6)
C8D	5357(3)	5645(3)	6339(3)	30.2(7)
C6C	8461(3)	10019(2)	3907(3)	29.2(7)
C5A	4024(3)	8863(3)	-936(3)	34.2(7)
C2D	8073(3)	4337(3)	7812(3)	31.8(7)
C7D	9369(3)	4760(3)	8401(3)	37.4(8)
C8B	9625(3)	6369(3)	3564(3)	30.5(7)
C4B	7965(4)	3713(3)	2827(4)	48.4(10)
C6D	6124(3)	4776(3)	6829(3)	29.0(6)
C2B	6651(3)	5019(3)	2069(3)	28.3(6)
C8C	8514(3)	9962(3)	2786(3)	36.7(8)
C4C	8739(4)	10839(3)	5759(4)	48(1)
C3D	7693(4)	3330(3)	7753(4)	45.3(9)
C5C	8827(3)	10892(3)	4765(4)	40.1(9)
C5B	8921(3)	4451(3)	3286(4)	40.8(9)
C5D	5677(4)	3792(3)	6757(4)	41.3(9)
C3C	8294(3)	9921(3)	5866(3)	41.3(9)
C3B	6818(4)	3995(3)	2202(4)	41.3(9)
O5S	10821(7)	10347(6)	9449(6)	168(3)
C4D	6485(4)	3064(3)	7236(4)	50.8(10)
O4S	4425(6)	8591(4)	5189(4)	124(2)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-La-II. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	21.16(5)	24.19(6)	16.54(5)	3.03(4)	9.14(4)	-2.69(4)
La1	24.02(8)	29.10(9)	21.07(8)	3.76(7)	13.23(7)	-1.59(6)
O71A	28.1(11)	39.9(13)	22.1(10)	8.2(9)	13.0(9)	8.9(9)
O71D	26.2(11)	45.2(15)	43.0(14)	16.8(12)	12.9(10)	9.7(10)
O81A	34.2(12)	36.7(13)	26.8(11)	0.5(10)	16.1(10)	4.2(10)
O72C	59.2(17)	50.9(17)	31.0(13)	14.0(12)	30.5(13)	8.4(13)
O71C	48.3(14)	29.2(12)	27.3(12)	1.7(9)	22.9(11)	-8.5(10)
O71B	26.2(11)	28.3(12)	33.6(12)	3.1(10)	12.6(9)	-1.6(9)
O81D	25.2(11)	35.4(13)	32.6(12)	10(1)	10.2(9)	0.7(9)
O72B	27.4(12)	35.9(14)	47.2(15)	0.1(11)	15.0(11)	-9.3(10)
O72A	41.9(14)	52.3(16)	31.4(13)	8.4(11)	27.3(11)	8.1(12)
N1A	22.0(11)	24.6(12)	21.2(11)	4.5(10)	10.9(9)	0.7(9)
O82B	22.9(12)	58.1(18)	51.0(17)	12.4(14)	6.0(11)	-0.8(11)
O81C	46.6(14)	42.6(15)	30.6(12)	9.1(11)	20.8(11)	-11.4(12)
O81B	25.6(11)	36.0(13)	32.6(12)	1.4(10)	8.1(9)	-8.5(9)
O1W	51.9(16)	43.9(16)	38.2(14)	2.4(12)	27.9(13)	0.6(13)
O82A	33.2(13)	56.7(18)	43.8(15)	0.3(13)	21.7(12)	11.2(12)
N1D	28.2(13)	29.3(14)	26.4(13)	6.5(11)	15.7(11)	2.7(10)
O72D	44.7(16)	52.2(18)	57.5(18)	21.8(15)	16.9(14)	23.6(14)
N1C	22.8(11)	25.3(13)	20.9(12)	5.3(10)	7.5(9)	-2.0(9)

O2W	34.8(14)	46.4(17)	86(2)	29.4(16)	28.7(15)	-2.6(12)
N1B	22.4(11)	25.0(13)	22.1(12)	3.6(10)	10.6(10)	-1.6(9)
O4W	38.5(16)	90(3)	64(2)	-16(2)	15.6(15)	3.4(17)
O82D	22.6(11)	50.5(17)	58.9(18)	1.3(14)	13.0(12)	-6.2(11)
C6B	24.8(14)	36.3(18)	25.2(15)	6.7(13)	11.8(12)	1.2(12)
O3S	98(3)	54(2)	71(2)	3.4(17)	60(2)	9.8(19)
O2S	40.8(15)	54.9(19)	59.6(19)	11.8(15)	17.1(14)	11.2(13)
O82C	57.2(19)	54.7(19)	64(2)	29.7(16)	19.8(16)	-22.5(15)
O3W	111(3)	48.5(19)	50.6(19)	14.1(15)	53(2)	23.9(19)
C7A	25.4(14)	28.1(15)	21.4(13)	2.6(11)	12.6(11)	-2.6(11)
O6S	32.4(14)	55.6(19)	65(2)	11.5(16)	11.8(14)	-1.4(13)
C6A	25.1(14)	24.7(15)	26.5(15)	2.2(12)	12.1(12)	0.6(11)
C2A	25.2(13)	23.0(14)	24.2(14)	4.7(11)	12.1(11)	-1.7(11)
C8A	28.5(15)	24.2(15)	33.7(17)	-1.6(13)	16.7(13)	-0.1(12)
C3A	34.1(16)	33.6(17)	23.5(15)	7.8(13)	12.9(13)	1.3(13)
C7C	30.9(15)	33.0(17)	22.9(14)	6.9(12)	14.2(12)	1.9(12)
C2C	25.8(14)	30.5(16)	24.6(14)	1.7(12)	11.7(12)	-0.8(12)
C4A	38.5(18)	36.7(19)	27.2(16)	13.3(14)	8.6(14)	7.1(15)
O1S	38.0(16)	95(3)	57(2)	12.3(19)	14.1(15)	1.9(17)
C7B	24.4(14)	30.4(16)	28.2(15)	1.7(13)	13.9(12)	-3.7(12)
C8D	24.8(14)	38.4(18)	25.1(15)	-0.1(13)	12.0(12)	-1.8(13)
C6C	21.5(13)	23.5(15)	34.5(16)	8.0(13)	6.9(12)	-1.8(11)
C5A	29.1(15)	32.2(18)	32.6(17)	6.1(14)	8.4(13)	8.4(13)
C2D	38.1(17)	32.2(17)	29.0(16)	10.1(13)	18.2(14)	6.7(14)
C7D	33.9(17)	49(2)	30.0(17)	12.5(16)	14.9(14)	13.5(15)
C8B	23.1(14)	40.1(19)	24.6(15)	6.0(13)	8.7(12)	-1.1(13)
C4B	46(2)	34(2)	75(3)	22(2)	34(2)	8.6(16)
C6D	31.4(15)	32.3(17)	26.6(15)	3.9(13)	17.1(13)	-2.3(13)
C2B	27.6(15)	28.6(16)	32.2(16)	4.6(13)	17.5(13)	-1.7(12)
C8C	24.7(15)	38.6(19)	42.4(19)	19.9(16)	9.8(14)	-5.1(13)
C4C	45(2)	32(2)	54(3)	-13.1(18)	19.7(19)	-2.9(16)
C3D	59(3)	34(2)	45(2)	14.6(17)	26(2)	10.3(18)
C5C	32.4(17)	23.3(16)	53(2)	0.9(15)	13.5(16)	-3.6(13)
C5B	35.2(18)	40(2)	50(2)	18.0(17)	20.7(17)	10.1(15)
C5D	47(2)	39(2)	41(2)	1.6(16)	24.7(17)	-9.9(16)
C3C	41.3(19)	45(2)	33.5(19)	-8.9(16)	19.4(16)	-3.8(16)
C3B	41(2)	28.4(18)	60(3)	9.3(17)	28.9(19)	-2.6(14)
O5S	204(7)	186(7)	113(5)	-68(5)	102(5)	-61(6)
C4D	69(3)	32(2)	57(3)	10.9(19)	35(2)	-2.9(19)
O4S	173(6)	91(4)	79(3)	-1(3)	45(3)	-55(4)

Table 4 Bond Lengths for U-La-II.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O71A	2.370(2)		N1D	C2D	1.343(4)
U1	O81A	2.399(2)		N1D	C6D	1.338(4)
U1	O71C	2.422(2)		O72D	C7D	1.265(4)

U1	O71B	2.338(2)		N1C	C2C	1.336(4)
U1	N1A	2.543(2)		N1C	C6C	1.336(4)
U1	O81C	2.397(2)		N1B	C6B	1.340(4)
U1	O81B	2.375(2)		N1B	C2B	1.330(4)
U1	N1C	2.555(3)		O82D	C8D	1.266(4)
U1	N1B	2.513(3)		C6B	C8B	1.507(5)
La1	O71D	2.482(2)		C6B	C5B	1.386(5)
La1	O72C	2.499(3)		O82C	C8C	1.228(4)
La1	O81D	2.520(2)		C7A	C2A	1.511(4)
La1	O72A[1]	2.482(2)		C6A	C8A	1.513(5)
La1	O1W	2.620(3)		C6A	C5A	1.388(4)
La1	N1D	2.620(3)		C2A	C3A	1.387(4)
La1	O2W	2.540(3)		C3A	C4A	1.392(5)
La1	O4W	2.715(3)		C7C	C2C	1.492(5)
La1	O3W	2.567(3)		C2C	C3C	1.393(5)
O71A	C7A	1.267(4)		C4A	C5A	1.379(5)
O71D	C7D	1.250(5)		C7B	C2B	1.507(5)
O81A	C8A	1.270(4)		C8D	C6D	1.508(5)
O72C	C7C	1.243(4)		C6C	C8C	1.507(5)
O71C	C7C	1.265(4)		C6C	C5C	1.378(5)
O71B	C7B	1.282(4)		C2D	C7D	1.512(5)
O81D	C8D	1.243(4)		C2D	C3D	1.376(5)
O72B	C7B	1.236(4)		C4B	C5B	1.376(6)
O72A	La1[2]	2.481(2)		C4B	C3B	1.377(6)
O72A	C7A	1.226(4)		C6D	C5D	1.374(5)
N1A	C6A	1.330(4)		C2B	C3B	1.376(5)
N1A	C2A	1.338(4)		C4C	C5C	1.383(6)
O82B	C8B	1.236(4)		C4C	C3C	1.379(6)
O81C	C8C	1.273(5)		C3D	C4D	1.375(6)
O81B	C8B	1.276(4)		C5D	C4D	1.387(6)
O82A	C8A	1.234(4)				

[1]+X,+Y,1+Z; [2]+X,+Y,-1+Z

II.15 U-Ce-II

Table 1 Crystal data and structure refinement for U-Ce-II.	
Identification code	U-Ce-II
Empirical formula	$C_{28}H_{20}CeN_4O_{26}U$
Formula weight	1206.63
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	12.8314(10)
b/Å	12.9942(10)
c/Å	13.1631(10)
α/°	98.258(4)

β/°	119.065(3)
γ/°	90.087(3)
Volume/Å^3	1892.0(3)
Z	2
ρ_{calc}g/cm^3	2.118
μ/mm^{-1}	5.566
F(000)	1148.0
Crystal size/mm^3	0.262 × 0.191 × 0.149
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.178 to 61.056
Index ranges	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -18 ≤ l ≤ 18
Reflections collected	70985
Independent reflections	11522 [R_{int} = 0.0244, R_{sigma} = 0.0150]
Data/restraints/parameters	11522/0/515
Goodness-of-fit on F^2	1.048
Final R indexes [I>=2σ (I)]	R_1 = 0.0205, wR_2 = 0.0537
Final R indexes [all data]	R_1 = 0.0221, wR_2 = 0.0545
Largest diff. peak/hole / e Å^{-3}	1.92/-0.89

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Ce-II. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	7179.3(2)	7608.7(2)	2297.5(2)	18.81(3)
Ce1	8070.3(2)	6939.0(2)	7530.8(2)	21.62(3)
O71A	7578.2(16)	7011.6(15)	743.2(15)	28.1(4)
O71D	9565.2(17)	5673.4(17)	8337.5(19)	36.0(4)
O81A	5597.6(16)	8652.9(15)	2180.2(16)	29.5(4)
O72C	7331(2)	7898.0(18)	5839.5(18)	38.9(5)
O71C	7124.2(19)	7357.5(15)	4058.1(16)	30.7(4)
O71B	5482.8(16)	6420.1(14)	1445.5(17)	29.0(4)
O81D	5858.8(16)	6476.6(15)	6370.6(17)	30.6(4)
O72B	4531.5(17)	4824.7(16)	973(2)	37.8(5)
O72A	7339.8(18)	6921.3(17)	-1055.9(17)	34.6(4)
N1A	5752.8(17)	8071.5(15)	289.9(17)	21.1(3)
O82B	10700.3(17)	6193.6(19)	4047(2)	43.7(5)
O81C	8085.0(19)	9121.9(17)	2079.1(18)	36.0(4)
O81B	9208.1(16)	7250.4(15)	3393.2(17)	31.1(4)
O1W	8028(2)	5759.1(18)	5739.2(19)	39.2(5)
O82A	3707.2(18)	9033.4(19)	1144(2)	42.2(5)
N1D	7301.7(19)	5037.3(16)	7357.0(19)	25.1(4)
O72D	10181(2)	4157(2)	8924(2)	50.3(6)
N1C	8019.9(17)	9134.7(15)	4014.0(17)	22.5(4)
O2W	9918.5(19)	7621.1(19)	7562(2)	46.9(6)
N1B	7572.7(17)	5735.6(15)	2522.4(17)	22.1(4)
O4W	9746(2)	7547(2)	9832(2)	47.4(5)

O82D	4244.3(18)	5462.3(19)	5919(2)	45.5(5)
C6B	8690(2)	5459(2)	3108(2)	26.4(5)
O3S	3790(3)	9853(2)	3233(3)	61.0(7)
O2S	7749(2)	4619(2)	188(2)	52.3(6)
O82C	8925(2)	10742(2)	2614(3)	59.5(8)
O3W	7853(3)	8838.1(19)	8134(2)	56.9(7)
C7A	7049(2)	7206.8(19)	-301(2)	23.1(4)
O6S	11826(2)	7414(2)	9699(2)	49.7(6)
C6A	4793(2)	8567.8(18)	134(2)	24.4(4)
C2A	5977(2)	7832.6(18)	-603(2)	22.0(4)
C8A	4666(2)	8769.4(19)	1227(2)	26.9(5)
C3A	5255(2)	8127(2)	-1692(2)	28.7(5)
C7C	7425(2)	8031(2)	4969(2)	25.4(4)
C2C	7939(2)	9075(2)	4980(2)	26.1(4)
C4A	4267(3)	8657(2)	-1848(2)	33.6(6)
O1S	6950(3)	2847(2)	4616(3)	63.2(7)
C7B	5443(2)	5431(2)	1432(2)	25.8(4)
C8D	5360(2)	5640(2)	6339(2)	28.6(5)
C6C	8459(2)	10027.2(19)	3921(2)	27.7(5)
C5A	4013(2)	8872(2)	-930(2)	32.1(5)
C2D	8078(2)	4326(2)	7814(2)	29.8(5)
C7D	9372(2)	4750(2)	8405(2)	33.7(6)
C8B	9629(2)	6358(2)	3561(2)	28.2(5)
C4B	7968(3)	3693(2)	2809(4)	45.7(8)
C6D	6128(2)	4768(2)	6829(2)	27.5(5)
C2B	6651(2)	5013.8(19)	2064(2)	26.1(5)
C8C	8510(2)	9979(2)	2797(3)	33.9(6)
C4C	8760(3)	10833(2)	5794(3)	46.1(8)
C3D	7699(3)	3306(2)	7747(3)	42.1(7)
C5C	8836(3)	10897(2)	4786(3)	38.4(6)
C5B	8928(3)	4441(2)	3277(3)	37.1(6)
C5D	5676(3)	3777(2)	6753(3)	39.4(6)
C3C	8307(3)	9912(2)	5895(3)	39.3(6)
C3B	6817(3)	3978(2)	2187(3)	39.9(7)
O5S	10780(5)	10420(4)	9432(5)	116.4(15)
C4D	6482(4)	3042(2)	7223(3)	48.0(8)
O4S	4458(5)	8582(4)	5198(4)	112.2(15)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Ce-II. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	18.70(4)	21.85(4)	15.48(4)	3.50(3)	7.99(3)	-1.01(3)
Ce1	22.30(6)	25.75(6)	20.08(6)	4.99(5)	12.62(5)	0.37(5)
O71A	26.8(8)	39.2(10)	20.9(8)	8.6(7)	12.8(7)	10.8(7)
O71D	25.4(9)	40.6(11)	40.8(11)	15.7(9)	12.9(8)	8.9(8)
O81A	28.5(8)	36.2(10)	23.4(8)	2.8(7)	12.9(7)	5.6(7)

O72C	53.3(13)	46.8(12)	27.0(9)	11.9(9)	26.2(9)	7.6(10)
O71C	44.6(11)	27.1(9)	25.8(9)	2.7(7)	21.9(8)	-5.2(8)
O71B	24.4(8)	26.7(8)	32.8(9)	2.7(7)	12.3(7)	-1.8(7)
O81D	23.6(8)	33.4(9)	30.6(9)	8.6(7)	9.2(7)	1.7(7)
O72B	25.1(9)	34.3(10)	47.3(12)	0.7(9)	14.2(8)	-8.3(8)
O72A	37.1(10)	49.3(12)	27.7(9)	7.6(8)	23.5(8)	6.3(9)
N1A	20.5(8)	22.8(9)	19.2(8)	3.6(7)	9.1(7)	1.7(7)
O82B	20.2(9)	51.1(13)	46.3(12)	9.7(10)	5.3(8)	2.1(8)
O81C	40.8(11)	39.9(11)	31.6(10)	11.4(8)	19.8(9)	-7.4(8)
O81B	23.2(8)	30.2(9)	31.2(9)	2.2(7)	7.4(7)	-5.9(7)
O1W	47.0(12)	40.2(11)	35.5(11)	3.6(9)	25(1)	3.8(9)
O82A	28.6(9)	55.9(14)	41.8(12)	0.8(10)	19.0(9)	11.3(9)
N1D	26.0(9)	26.2(10)	26.4(10)	6.5(8)	14.8(8)	3.0(8)
O72D	43.3(12)	48.5(13)	54.8(14)	23.2(11)	16.9(11)	24.6(11)
N1C	20.5(8)	21.9(9)	21.4(9)	4.8(7)	7.2(7)	-1.5(7)
O2W	31.5(10)	45.1(12)	67.3(16)	26.5(11)	22.2(11)	-2.8(9)
N1B	20.7(8)	23.6(9)	21.7(9)	3.5(7)	10.3(7)	-0.5(7)
O4W	39.5(12)	54.0(14)	46.4(13)	8.0(11)	19.5(10)	2.2(10)
O82D	22.4(9)	48.4(13)	55.8(14)	1.5(11)	13.3(9)	-4.3(9)
C6B	22.4(10)	30.6(12)	25.0(11)	6.7(9)	10.1(9)	1.9(9)
O82C	52.1(14)	54.4(15)	65.8(17)	33.3(13)	18.1(13)	-18.3(12)
O3W	99(2)	40.6(13)	43.2(13)	11.9(10)	42.5(15)	22.2(13)
C7A	22.7(10)	27.8(11)	20.8(10)	4.2(8)	12.2(8)	0.3(8)
C6A	22.9(10)	22.8(10)	25.1(11)	3.5(8)	10.2(9)	2.1(8)
C2A	22.3(10)	24.5(10)	19.4(10)	4.8(8)	10.1(8)	-0.6(8)
C8A	27.2(11)	24.3(11)	29.8(12)	0.6(9)	15.5(9)	2.4(9)
C3A	31.2(12)	32.8(12)	21.1(10)	8.1(9)	11.1(9)	0.4(10)
C7C	27.5(11)	30.2(11)	20.8(10)	7.7(9)	12.8(9)	4.4(9)
C2C	24.3(10)	27.7(11)	22.8(10)	1.1(9)	9.6(9)	1.1(9)
C4A	34.4(13)	34.4(13)	23.9(11)	11.2(10)	6.3(10)	6.2(11)
C7B	22(1)	28.6(11)	26.4(11)	-0.3(9)	12.9(9)	-4.2(9)
C8D	23.6(11)	33.6(12)	25.9(11)	-0.3(9)	11.5(9)	-1.2(9)
C6C	19.2(10)	21.4(10)	34.2(12)	7.4(9)	6.0(9)	-0.7(8)
C5A	27.2(12)	31.6(12)	31.2(13)	8.2(10)	8.6(10)	9.4(10)
C2D	35.4(13)	29.5(12)	27.6(12)	9.9(10)	16.5(10)	7.3(10)
C7D	29.5(12)	41.5(15)	30.8(13)	12.6(11)	13.6(10)	13.8(11)
C8B	20.5(10)	35.3(13)	23.6(11)	4.4(9)	7.2(9)	-0.1(9)
C4B	44.4(17)	28.6(13)	72(2)	20.6(15)	31.9(17)	8.3(12)
C6D	29.8(12)	28.3(11)	27.7(11)	3.1(9)	17.1(10)	-1.4(9)
C2B	25.4(11)	25.3(11)	29.0(11)	2.8(9)	14.9(9)	-2.1(9)
C8C	22.4(11)	35.0(13)	39.7(14)	19.8(11)	8.2(10)	-3.9(10)
C4C	44.3(17)	31.1(14)	50.1(19)	-13.7(13)	18.6(14)	-3.8(12)
C3D	57.7(19)	29.7(13)	39.1(15)	13.0(12)	21.9(14)	9.1(13)
C5C	29.8(13)	20.8(11)	51.6(17)	0.8(11)	11.3(12)	-2.7(10)
C5B	30.0(13)	36.5(14)	46.0(16)	15.8(12)	17.3(12)	8.7(11)
C5D	44.2(16)	34.5(14)	40.8(15)	1.0(12)	23.3(13)	-9.7(12)
C3C	38.3(14)	40.6(15)	32.4(14)	-8.9(12)	16.3(12)	-2.3(12)
C3B	37.1(14)	25.3(12)	61(2)	8.4(12)	26.3(14)	-3.1(11)

C4D	67(2)	27.8(14)	50.6(19)	7.5(13)	29.3(17)	-6.6(14)

Table 4 Bond Lengths for U-Ce-II.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O71A	2.3691(17)		N1D	C2D	1.337(3)
U1	O81A	2.3976(18)		N1D	C6D	1.336(3)
U1	O71C	2.4205(18)		O72D	C7D	1.266(3)
U1	O71B	2.3457(18)		N1C	C2C	1.337(3)
U1	N1A	2.5409(19)		N1C	C6C	1.336(3)
U1	O81C	2.4042(19)		N1B	C6B	1.336(3)
U1	O81B	2.3711(19)		N1B	C2B	1.336(3)
U1	N1C	2.557(2)		O82D	C8D	1.266(3)
U1	N1B	2.516(2)		C6B	C8B	1.506(4)
Ce1	O71D	2.4583(19)		C6B	C5B	1.384(4)
Ce1	O72C	2.481(2)		O82C	C8C	1.231(3)
Ce1	O81D	2.5033(18)		C7A	C2A	1.509(3)
Ce1	O72A[1]	2.4590(18)		C6A	C8A	1.512(4)
Ce1	O1W	2.599(2)		C6A	C5A	1.385(3)
Ce1	N1D	2.597(2)		C2A	C3A	1.388(3)
Ce1	O2W	2.510(2)		C3A	C4A	1.384(4)
Ce1	O4W	2.721(2)		C7C	C2C	1.502(4)
Ce1	O3W	2.540(2)		C2C	C3C	1.388(4)
O71A	C7A	1.268(3)		C4A	C5A	1.389(4)
O71D	C7D	1.250(4)		C7B	C2B	1.506(4)
O81A	C8A	1.274(3)		C8D	C6D	1.505(4)
O72C	C7C	1.244(3)		C6C	C8C	1.505(4)
O71C	C7C	1.265(3)		C6C	C5C	1.379(4)
O71B	C7B	1.283(3)		C2D	C7D	1.512(4)
O81D	C8D	1.246(3)		C2D	C3D	1.387(4)
O72B	C7B	1.236(3)		C4B	C5B	1.389(4)
O72A	Ce1[2]	2.4590(18)		C4B	C3B	1.379(5)
O72A	C7A	1.233(3)		C6D	C5D	1.382(4)
N1A	C6A	1.331(3)		C2B	C3B	1.383(4)
N1A	C2A	1.336(3)		C4C	C5C	1.390(5)
O82B	C8B	1.237(3)		C4C	C3C	1.381(5)
O81C	C8C	1.275(4)		C3D	C4D	1.384(5)
O81B	C8B	1.283(3)		C5D	C4D	1.385(5)
O82A	C8A	1.234(3)				

[1]+X,+Y,1+Z; [2]+X,+Y,-1+Z

II.16 U-Ce-III

Table 1 Crystal data and structure refinement for U-Ce-III.	
Identification code	U-Ce-III
Empirical formula	$C_{98}H_{58}Ce_4N_{14}O_{86}U_4$
Formula weight	4320.18
Temperature/K	299.29
Crystal system	triclinic
Space group	P-1
a/Å	14.931(2)
b/Å	15.195(2)
c/Å	17.586(3)
α/°	105.231(8)
β/°	100.564(8)
γ/°	101.090(7)
Volume/Å^3	3660.9(10)
Z	1
ρ_{calc}g/cm^3	1.960
μ/mm^{-1}	5.732
F(000)	2032.0
Crystal size/mm^3	0.233 × 0.146 × 0.136
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.868 to 56.616
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -23 ≤ l ≤ 23
Reflections collected	210842
Independent reflections	18016 [R_{int} = 0.0425, R_{sigma} = 0.0230]
Data/restraints/parameters	18016/0/932
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0436, wR_2 = 0.1263
Final R indexes [all data]	R_1 = 0.0514, wR_2 = 0.1316
Largest diff. peak/hole / e Å^{-3}	4.07/-5.35

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Ce-III. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	2356.1(2)	2097.0(2)	4456.7(2)	25.42(6)
U2	2737.3(2)	2020.8(2)	-361.4(2)	26.41(6)
Ce1	79.1(2)	3746.2(2)	1849.8(2)	27.78(8)
Ce2	3235.5(4)	7761.3(6)	4394.9(3)	68.43(19)
O71A	2450(4)	953(3)	5177(3)	37.3(11)
O71B	2345(3)	714(4)	3463(3)	36.7(10)
O81E	1875(4)	2138(3)	-1571(3)	39.0(11)
O81F	1570(3)	2604(3)	297(3)	33.4(10)
O81C	1521(3)	2510(4)	3342(3)	38.8(11)

O82F	200(3)	2395(4)	657(3)	38.9(11)
O71G	-877(4)	3866(3)	596(3)	37.9(11)
O71C	4013(3)	2137(4)	4769(3)	39.3(11)
O71E	3712(4)	3283(4)	725(3)	39.0(11)
O81A	2819(4)	3749(3)	5005(3)	43.6(12)
O71D	3999(4)	2276(4)	-988(3)	40.1(11)
N1C	3317(4)	2662(4)	3549(3)	31.1(11)
N1A	3041(4)	2747(4)	5972(3)	30.8(11)
O81B	1067(4)	2464(4)	4960(3)	45.3(13)
O1W	1512(4)	4338(3)	1292(3)	37.1(10)
O81D	2673(4)	1267(4)	650(3)	45.3(13)
N1G	147(4)	5414(4)	1712(3)	30.0(11)
O81G	1079(4)	5133(4)	3025(3)	46.2(13)
N1D	4206(4)	1514(4)	161(4)	36.3(12)
N1F	1100(4)	898(4)	-713(3)	28.6(10)
O71F	2517(4)	474(3)	-1280(3)	41.0(11)
O82C	1431(4)	3074(4)	2298(3)	48.6(14)
O3W	-1127(4)	4390(4)	2492(4)	51.1(14)
O2W	-121(5)	3141(5)	3059(4)	56.8(16)
O72G	-1414(4)	4630(4)	-239(3)	40.4(11)
C6F	422(5)	1163(4)	-389(4)	30.2(12)
O72F	1673(6)	-976(4)	-2036(4)	66.0(19)
C7G	-923(5)	4601(5)	407(4)	32.0(13)
C7F	1750(6)	-181(5)	-1557(5)	41.2(16)
C6C	2906(5)	2908(5)	2922(4)	35.7(14)
C8C	1872(5)	2830(5)	2840(4)	35.7(14)
O82G	1736(5)	6682(4)	3602(4)	67(2)
O11W	1991(5)	8722(5)	4499(5)	68.1(19)
C2G	-327(4)	5522(4)	1039(4)	28.3(12)
N1B	804(4)	852(4)	3907(3)	30.5(11)
O72B	1709(5)	-754(4)	2633(4)	56.7(16)
C2B	749(5)	32(5)	3354(4)	32.8(13)
O82B	-381(5)	2160(5)	5132(5)	80(3)
C7B	1658(5)	-29(5)	3112(4)	32.9(13)
C6B	57(5)	1001(5)	4177(5)	41.2(16)
N1E	2925(4)	3665(4)	-517(3)	30.0(11)
C6E	2500(5)	3779(5)	-1215(4)	32.6(13)
C7E	3952(6)	4158(5)	791(4)	41.7(16)
C2E	3510(5)	4411(5)	58(4)	35.7(14)
C5F	-493(5)	607(5)	-619(5)	39.2(15)
C3F	18(6)	-565(5)	-1528(5)	43.3(17)
C4F	-707(6)	-244(6)	-1202(5)	47.0(18)
O72E	4471(6)	4775(5)	1389(4)	86(3)
C8B	239(5)	1942(6)	4808(5)	45.8(18)
C2A	3201(5)	2163(5)	6402(4)	32.1(13)
C7A	2865(5)	1133(5)	5916(4)	33.7(14)
C6A	3348(5)	3681(5)	6322(4)	39.0(16)
O82E	1488(5)	2841(4)	-2498(3)	56.7(16)

O72D	5468(5)	2349(5)	-1111(4)	61.7(17)
C7D	4821(5)	2138(5)	-794(5)	39.4(15)
C5E	2647(6)	4646(5)	-1347(5)	45.8(18)
C8E	1898(5)	2860(5)	-1831(4)	36.9(15)
C4E	3239(7)	5415(5)	-744(6)	54(2)
C6D	4235(6)	1135(6)	765(5)	47.2(18)
C2D	4966(5)	1702(6)	-122(5)	40.8(16)
C4A	4000(7)	3449(7)	7585(5)	55(2)
C3G	-260(5)	6387(5)	916(5)	38.9(15)
C6G	688(5)	6177(5)	2296(4)	35.1(14)
C8G	1211(6)	5989(6)	3036(5)	46.5(18)
C5G	793(6)	7075(5)	2228(5)	47.7(19)
C4G	316(6)	7182(5)	1520(5)	44.2(17)
O72A	3015(4)	539(4)	6248(4)	48.9(13)
O82A	3305(6)	5106(4)	6011(5)	77(2)
C8A	3149(6)	4243(5)	5764(5)	44.1(17)
C3A	3679(6)	2499(6)	7218(4)	50(2)
C5A	3840(7)	4060(6)	7141(5)	54(2)
O72C	5468(4)	2457(6)	4592(4)	67(2)
C7C	4627(5)	2420(6)	4404(5)	41.8(17)
C2C	4246(5)	2716(6)	3684(5)	39.7(16)
C5C	3421(6)	3217(7)	2412(5)	56(2)
C3E	3699(6)	5303(5)	-21(5)	49.1(19)
C8D	3327(6)	986(7)	1024(6)	56(2)
C3C	4786(6)	3008(8)	3201(6)	61(3)
C3B	-67(6)	-678(6)	3062(5)	52(2)
C4C	4362(7)	3254(9)	2555(6)	70(3)
C5B	-802(6)	333(7)	3891(6)	62(3)
C2F	912(5)	47(4)	-1265(4)	34.2(14)
O82D	3251(7)	615(9)	1567(6)	112(4)
O7W	2471(7)	7246(9)	5372(6)	121(4)
O8W	4867(7)	8517(10)	4241(7)	128(5)
C3D	5802(6)	1522(8)	204(6)	61(2)
O10W	3886(6)	9124(7)	5706(6)	100(3)
C4D	5832(7)	1114(10)	818(7)	80(4)
C5D	5028(7)	917(9)	1115(7)	69(3)
O6W	3026(8)	8021(10)	3056(7)	145(5)
O4W	-1422(4)	2447(4)	1397(4)	54.3(15)
C8F	736(4)	2129(4)	246(4)	30.2(13)
C4B	-858(7)	-520(8)	3332(7)	73(3)
O5S	-2933(7)	3609(7)	2601(6)	38(2)
O3S	3755(7)	58(7)	-2303(6)	33.9(19)
O6S	-929(7)	6131(7)	3470(6)	40(2)
O8S	4717(10)	8785(9)	2738(8)	60(3)
O4S	2807(8)	-1859(8)	-2963(7)	46(2)
O1S	-2091(10)	1952(10)	-277(9)	66(3)
O2S	-2795(11)	3143(11)	-1431(10)	74(4)
O7S	4198(9)	10497(9)	3085(8)	54(3)

O9W	3583(18)	9643(16)	4237(19)	272(12)
O5W	3853(12)	6490(12)	3814(10)	99(7)
O9S	2869(18)	5729(17)	4395(15)	126(8)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Ce-III. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	23.31(11)	26.21(11)	24.24(11)	7.57(8)	1.85(8)	4.69(8)
U2	25.57(11)	24.79(11)	28.80(12)	10.37(9)	5.08(9)	4.85(8)
Ce1	30.10(17)	27.04(17)	31.29(18)	14.88(14)	7.05(13)	11.38(13)
Ce2	38.7(2)	132.3(6)	34.2(2)	11.2(3)	4.24(19)	46.0(3)
O71A	47(3)	28(2)	28(2)	6.2(19)	1(2)	0(2)
O71B	35(2)	39(3)	32(2)	5(2)	9(2)	8(2)
O81E	45(3)	28(2)	34(3)	8(2)	-6(2)	1(2)
O81F	29(2)	28(2)	41(3)	7.0(19)	9.7(19)	6.8(18)
O81C	32(2)	52(3)	40(3)	26(2)	6(2)	17(2)
O82F	34(2)	38(3)	45(3)	9(2)	13(2)	11(2)
O71G	45(3)	30(2)	38(3)	16(2)	1(2)	10(2)
O71C	29(2)	60(3)	35(3)	25(2)	3.3(19)	12(2)
O71E	42(3)	38(3)	29(2)	12(2)	-1(2)	-1(2)
O81A	53(3)	29(2)	44(3)	12(2)	6(2)	5(2)
O71D	40(3)	54(3)	38(3)	26(2)	17(2)	14(2)
N1C	26(3)	38(3)	30(3)	15(2)	4(2)	7(2)
N1A	28(3)	28(3)	29(3)	4(2)	4(2)	-1(2)
O81B	33(3)	39(3)	49(3)	-9(2)	12(2)	4(2)
O1W	40(3)	33(2)	40(3)	16(2)	11(2)	8(2)
O81D	39(3)	60(3)	51(3)	36(3)	17(2)	15(2)
N1G	36(3)	28(3)	28(3)	11(2)	4(2)	11(2)
O81G	61(3)	39(3)	34(3)	12(2)	-5(2)	18(3)
N1D	29(3)	44(3)	40(3)	20(3)	7(2)	10(2)
N1F	31(3)	21(2)	32(3)	9(2)	5(2)	3(2)
O71F	44(3)	28(2)	50(3)	6(2)	17(2)	9(2)
O82C	48(3)	69(4)	43(3)	32(3)	7(2)	32(3)
O3W	53(3)	42(3)	64(4)	13(3)	25(3)	21(3)
O2W	63(4)	75(4)	57(4)	42(3)	24(3)	37(3)
O72G	45(3)	41(3)	36(3)	19(2)	0(2)	11(2)
C6F	32(3)	28(3)	30(3)	11(2)	4(2)	7(2)
O72F	93(5)	25(3)	77(5)	2(3)	43(4)	8(3)
C7G	34(3)	36(3)	32(3)	14(3)	9(3)	16(3)
C7F	57(5)	25(3)	45(4)	10(3)	20(4)	11(3)
C6C	34(3)	42(4)	30(3)	16(3)	2(3)	9(3)
C8C	40(4)	39(4)	30(3)	12(3)	3(3)	18(3)
O82G	90(5)	46(3)	40(3)	2(3)	-23(3)	11(3)
O11W	50(4)	73(5)	79(5)	14(4)	16(3)	22(3)
C2G	30(3)	27(3)	32(3)	13(2)	7(2)	13(2)
N1B	24(2)	31(3)	30(3)	3(2)	2(2)	5(2)

O72B	60(4)	40(3)	60(4)	-6(3)	20(3)	14(3)
C2B	33(3)	29(3)	32(3)	7(3)	6(3)	6(3)
O82B	43(4)	71(5)	99(6)	-23(4)	32(4)	4(3)
C7B	37(3)	30(3)	30(3)	7(3)	7(3)	10(3)
C6B	31(3)	42(4)	42(4)	0(3)	10(3)	4(3)
N1E	29(3)	28(3)	29(3)	8(2)	2(2)	3(2)
C6E	34(3)	31(3)	32(3)	12(3)	5(3)	6(3)
C7E	44(4)	39(4)	31(3)	7(3)	2(3)	-6(3)
C2E	39(4)	26(3)	34(3)	8(3)	2(3)	-2(3)
C5F	33(3)	35(4)	48(4)	14(3)	8(3)	4(3)
C3F	46(4)	29(3)	42(4)	7(3)	4(3)	-6(3)
C4F	38(4)	42(4)	49(4)	12(3)	1(3)	-5(3)
O72E	108(6)	53(4)	51(4)	9(3)	-31(4)	-27(4)
C8B	34(4)	43(4)	48(4)	-5(3)	12(3)	5(3)
C2A	31(3)	38(3)	23(3)	7(3)	6(2)	3(3)
C7A	34(3)	39(4)	30(3)	16(3)	10(3)	4(3)
C6A	44(4)	29(3)	33(3)	-2(3)	10(3)	-1(3)
O82E	68(4)	50(3)	37(3)	17(3)	-15(3)	4(3)
O72D	50(3)	80(5)	67(4)	31(4)	33(3)	14(3)
C7D	34(3)	42(4)	42(4)	9(3)	17(3)	5(3)
C5E	54(5)	39(4)	47(4)	21(3)	7(4)	13(3)
C8E	38(4)	34(3)	34(3)	10(3)	0(3)	6(3)
C4E	69(6)	25(3)	66(6)	21(4)	10(4)	5(3)
C6D	43(4)	62(5)	50(5)	33(4)	14(3)	20(4)
C2D	31(3)	49(4)	43(4)	14(3)	11(3)	12(3)
C4A	65(6)	55(5)	27(4)	3(3)	-3(4)	0(4)
C3G	46(4)	33(3)	42(4)	19(3)	6(3)	16(3)
C6G	41(4)	30(3)	34(3)	11(3)	3(3)	14(3)
C8G	61(5)	42(4)	34(4)	11(3)	-2(3)	20(4)
C5G	62(5)	28(3)	48(4)	10(3)	-1(4)	14(3)
C4G	58(5)	29(3)	46(4)	14(3)	5(4)	17(3)
O72A	58(3)	47(3)	46(3)	26(3)	7(3)	11(3)
O82A	112(6)	26(3)	78(5)	5(3)	15(4)	3(3)
C8A	43(4)	27(3)	51(4)	4(3)	6(3)	0(3)
C3A	57(5)	57(5)	25(3)	10(3)	0(3)	1(4)
C5A	59(5)	42(4)	38(4)	-3(3)	0(4)	-6(4)
O72C	30(3)	131(6)	56(4)	53(4)	8(3)	27(3)
C7C	27(3)	63(5)	38(4)	23(4)	4(3)	11(3)
C2C	28(3)	55(4)	38(4)	21(3)	6(3)	8(3)
C5C	48(5)	86(7)	41(4)	40(5)	8(4)	12(4)
C3E	60(5)	27(3)	49(5)	6(3)	8(4)	-3(3)
C8D	52(5)	80(6)	62(5)	53(5)	22(4)	25(4)
C3C	34(4)	104(8)	56(5)	46(5)	13(4)	11(4)
C3B	46(4)	38(4)	53(5)	-7(3)	12(4)	-2(3)
C4C	46(5)	115(9)	61(6)	53(6)	18(4)	7(5)
C5B	37(4)	63(6)	64(6)	-10(5)	18(4)	-2(4)
C2F	43(4)	22(3)	36(3)	12(3)	7(3)	2(3)
O82D	92(6)	197(11)	129(8)	145(8)	55(6)	67(7)

O7W	94(7)	152(10)	80(6)	49(6)	-9(5)	-41(7)
O8W	82(6)	249(14)	142(9)	151(10)	60(6)	91(8)
C3D	38(4)	84(7)	70(6)	31(5)	19(4)	23(4)
O10W	78(6)	89(6)	104(7)	1(5)	-11(5)	29(5)
C4D	49(5)	138(11)	83(8)	63(8)	19(5)	52(7)
C5D	56(6)	100(8)	73(7)	51(6)	12(5)	39(6)
O6W	107(8)	198(13)	98(8)	89(8)	-25(6)	-43(8)
O4W	51(3)	49(3)	68(4)	24(3)	23(3)	7(3)
C8F	29(3)	28(3)	35(3)	10(3)	5(3)	11(2)
C4B	43(5)	68(6)	72(7)	-16(5)	18(5)	-20(4)
O9W	250(30)	210(20)	410(40)	130(20)	130(30)	108(19)
O5W	93(12)	89(11)	85(11)	-30(9)	-11(9)	69(10)

Table 4 Bond Lengths for U-Ce-III.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O71A	2.414(5)		O82C	C8C	1.237(8)
U1	O71B	2.348(5)		O72G	C7G	1.250(8)
U1	O81C	2.417(5)		C6F	C5F	1.385(9)
U1	O71C	2.420(5)		C6F	C8F	1.517(9)
U1	O81A	2.350(5)		O72F	C7F	1.248(9)
U1	N1C	2.535(5)		C7G	C2G	1.525(9)
U1	N1A	2.520(5)		C7F	C2F	1.502(11)
U1	O81B	2.362(5)		C6C	C8C	1.503(10)
U1	N1B	2.533(5)		C6C	C5C	1.397(11)
U2	O81E	2.345(5)		O82G	C8G	1.249(10)
U2	O81F	2.441(5)		C2G	C3G	1.376(9)
U2	O71E	2.330(5)		N1B	C2B	1.341(8)
U2	O71D	2.371(5)		N1B	C6B	1.326(9)
U2	O81D	2.361(5)		O72B	C7B	1.223(8)
U2	N1D	2.556(6)		C2B	C7B	1.508(9)
U2	N1F	2.561(5)		C2B	C3B	1.374(10)
U2	O71F	2.399(5)		O82B	C8B	1.226(9)
U2	N1E	2.552(5)		C6B	C8B	1.501(10)
Ce1	O82F	2.582(5)		C6B	C5B	1.386(11)
Ce1	O71G	2.467(5)		N1E	C6E	1.345(8)
Ce1	O1W	2.616(5)		N1E	C2E	1.327(8)
Ce1	N1G	2.593(5)		C6E	C5E	1.380(10)
Ce1	O81G	2.512(5)		C6E	C8E	1.515(9)
Ce1	O82C	2.525(5)		C7E	C2E	1.512(10)
Ce1	O3W	2.513(5)		C7E	O72E	1.221(9)
Ce1	O2W	2.571(6)		C2E	C3E	1.380(10)
Ce1	O4W	2.524(6)		C5F	C4F	1.360(11)
Ce2	O82G	2.427(7)		C3F	C4F	1.423(12)
Ce2	O11W	2.578(7)		C3F	C2F	1.389(10)
Ce2	O72C[1]	2.515(6)		C2A	C7A	1.506(10)
Ce2	O7W	2.438(10)		C2A	C3A	1.390(10)

Ce2	O8W	2.579(10)		C7A	O72A	1.230(8)
Ce2	O10W	2.538(9)		C6A	C8A	1.487(11)
Ce2	O6W	2.462(10)		C6A	C5A	1.400(11)
Ce2	O9W	2.90(2)		O82E	C8E	1.210(9)
Ce2	O5W	2.370(12)		O72D	C7D	1.234(9)
O71A	C7A	1.265(8)		C7D	C2D	1.502(11)
O71B	C7B	1.290(8)		C5E	C4E	1.371(12)
O81E	C8E	1.292(8)		C4E	C3E	1.398(13)
O81F	C8F	1.288(8)		C6D	C8D	1.502(12)
O81C	C8C	1.260(9)		C6D	C5D	1.372(12)
O82F	C8F	1.228(8)		C2D	C3D	1.384(11)
O71G	C7G	1.257(8)		C4A	C3A	1.364(12)
O71C	C7C	1.283(9)		C4A	C5A	1.387(13)
O71E	C7E	1.277(9)		C3G	C4G	1.384(11)
O81A	C8A	1.296(10)		C6G	C8G	1.513(10)
O71D	C7D	1.284(9)		C6G	C5G	1.383(10)
N1C	C6C	1.338(8)		C5G	C4G	1.383(11)
N1C	C2C	1.347(9)		O82A	C8A	1.228(9)
N1A	C2A	1.336(9)		O72C	Ce2[1]	2.515(5)
N1A	C6A	1.338(8)		O72C	C7C	1.224(9)
O81B	C8B	1.273(9)		C7C	C2C	1.504(10)
O81D	C8D	1.281(10)		C2C	C3C	1.369(11)
N1G	C2G	1.331(8)		C5C	C4C	1.367(13)
N1G	C6G	1.327(9)		C8D	O82D	1.241(10)
O81G	C8G	1.273(9)		C3C	C4C	1.373(13)
N1D	C6D	1.333(9)		C3B	C4B	1.390(13)
N1D	C2D	1.331(9)		C5B	C4B	1.382(13)
N1F	C6F	1.327(8)		C3D	C4D	1.377(14)
N1F	C2F	1.340(8)		C4D	C5D	1.406(15)
O71F	C7F	1.281(9)				

[1]1-X,1-Y,1-Z

II.17 U-Nd-III

Table 1 Crystal data and structure refinement for U-Nd-III.	
Identification code	U-Nd-III
Empirical formula	$C_{98}H_{86}N_{14}Nd_4O_{102}U_4$
Formula weight	4620.88
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	14.8944(16)
b/Å	15.1661(16)
c/Å	17.5494(17)
α/°	106.770(4)
β/°	100.779(4)

γ/°	100.871(5)
Volume/Å^3	3602.5(7)
Z	1
ρ_{calc}g/cm^3	2.130
μ/mm^{-1}	4.712
F(000)	2196.0
Crystal size/mm^3	0.248 × 0.204 × 0.151
Radiation	AgKα (λ = 0.56086)
2Θ range for data collection/°	1.978 to 43.974
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -23 ≤ l ≤ 23
Reflections collected	238074
Independent reflections	17854 [R_{int} = 0.0544, R_{sigma} = 0.0220]
Data/restraints/parameters	17854/0/1011
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0196, wR_2 = 0.0451
Final R indexes [all data]	R_1 = 0.0229, wR_2 = 0.0473
Largest diff. peak/hole / e Å^{-3}	2.18/-1.06

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Nd-III. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U2	2738.8(2)	2002.4(2)	-434.9(2)	5.40(2)
U1	7582.2(2)	7799.1(2)	5599.3(2)	5.90(2)
Nd2	3273.4(2)	7948.3(2)	4444.3(2)	7.62(3)
Nd1	119.5(2)	3762.8(2)	1805.1(2)	6.04(3)
O72A	7246.9(15)	9551.0(15)	3917.6(13)	11.4(4)
O72F	1706.0(17)	-1090.8(15)	-2056.4(15)	16.0(5)
O82E	1396.3(16)	2793.9(16)	-2562.8(13)	14.5(4)
O82C	8438.2(16)	6812.3(16)	7764.9(13)	13.8(4)
O4W	-1367.8(15)	2466.0(15)	1318.4(13)	12.4(4)
O72B	8167.2(16)	10765.4(15)	7323.5(14)	13.8(4)
O71G	-860.6(15)	3827.5(14)	554.2(13)	10.3(4)
O81G	1142.8(16)	5147.8(15)	3001.4(13)	12.7(4)
O10W	3891.7(16)	9162.6(16)	5858.1(14)	14.9(4)
O72D	5479.0(15)	2342.1(16)	-1183.5(13)	13.2(4)
O71D	3989.0(15)	2228.2(15)	-1075.7(13)	10.3(4)
O1W	1512.3(15)	4352.6(14)	1235.7(13)	9.7(4)
O82F	228.7(15)	2388.3(15)	619.5(13)	10.4(4)
O11W	1913.4(16)	8643.6(16)	4667.3(15)	16.4(5)
O6W	3046.6(16)	8027.3(16)	3007.4(13)	14.4(4)
O82A	6589(2)	4819.8(17)	3831.8(15)	24.0(6)
O00Q	4940.3(15)	8711.2(16)	4380.8(13)	12.4(4)
O72G	-1442.0(15)	4584.3(15)	-265.8(13)	9.9(4)
O82B	10401.1(17)	7640.7(16)	5078.8(16)	21.8(5)
O9W	3522.2(15)	9672.6(15)	4390.6(13)	11.5(4)
O82G	1857.6(16)	6704.0(15)	3600.8(14)	15.0(5)
O71E	3767.1(15)	3299.7(15)	667.0(13)	10.6(4)
N1C	6586.8(17)	7269.6(17)	6485.9(15)	8.2(5)

C2G	-326(2)	5503(2)	1021.7(17)	6.8(5)
O7W	2525.5(16)	7157.3(17)	5293.7(14)	17.7(5)
C4G	325(2)	7192(2)	1533.4(19)	10.3(6)
O2W	-33.6(17)	3171.8(18)	2974.2(16)	21.0(5)
C3G	-267(2)	6381(2)	909.8(18)	9.5(5)
O72C	4484.1(15)	7598.0(16)	5451.9(13)	13.0(4)
O81D	2687.5(15)	1248.6(15)	573.1(13)	11.8(4)
O71A	7577.3(15)	9023.8(14)	4975.5(13)	10.6(4)
O72E	4478.1(17)	4833.0(16)	1386.9(14)	18.7(5)
C5G	814(2)	7102(2)	2254.9(19)	10.3(6)
O82D	3242.0(17)	495.9(17)	1413.8(15)	18.2(5)
O5W	3877(2)	6628(2)	3774.2(17)	31.8(7)
N1D	4219.0(17)	1512.6(17)	90.5(15)	8.5(5)
C2A	6892(2)	7873(2)	3656.6(17)	7.9(5)
N1B	9143.7(17)	9038.1(17)	6211.0(15)	8.3(5)
C5B	10779(2)	9541(2)	6269(2)	14.8(6)
C5E	2579(2)	4646(2)	-1375.0(19)	12.7(6)
O81C	8378.2(15)	7341.4(16)	6692.1(13)	12.0(4)
C6G	734(2)	6197(2)	2307.8(18)	7.9(5)
O71B	7589.0(14)	9206.1(14)	6614.8(13)	9.3(4)
O3W	-1075.6(16)	4380.9(15)	2446.1(14)	13.5(4)
O81B	8894.6(15)	7377.2(15)	5141.9(13)	12.3(4)
N1F	1113.6(17)	847.4(17)	-779.6(15)	7.4(5)
C4D	5890(2)	1195(3)	797(2)	19.5(7)
C7G	-929.6(19)	4568(2)	381.9(17)	6.8(5)
C8E	1838(2)	2835(2)	-1883.2(18)	9.5(5)
C4F	-680(2)	-367(2)	-1227.3(19)	12.1(6)
C5D	5082(2)	957(2)	1063(2)	15.8(6)
O71C	5935.9(15)	7799.4(15)	5246.0(13)	10.8(4)
C7A	7264.2(19)	8898(2)	4205.6(18)	7.7(5)
O81F	1591.2(14)	2594.7(14)	239.9(13)	9.3(4)
O81A	7060.4(16)	6149.9(15)	4940.1(13)	14.2(4)
C2C	5671(2)	7269(2)	6349.5(18)	10.2(6)
C5F	-471(2)	542(2)	-649.4(19)	10.6(6)
C6A	6627(2)	6312(2)	3630.9(19)	10.8(6)
C4E	3198(2)	5440(2)	-752(2)	16.1(6)
C3C	5106(2)	7019(2)	6838(2)	14.9(6)
C3E	3672(2)	5330(2)	-35(2)	14.0(6)
C8G	1289(2)	6011(2)	3034.6(18)	10.2(6)
O71F	2506.8(15)	433.2(15)	-1386.5(13)	11.0(4)
C3F	35(2)	-671(2)	-1559.8(19)	11.5(6)
C7D	4829(2)	2131(2)	-867.2(18)	8.8(5)
C6B	9918(2)	8864(2)	5978.4(18)	10.2(6)
N1G	175.1(17)	5414.7(17)	1705.1(15)	7.0(4)
C8B	9748(2)	7885(2)	5354.3(19)	11.6(6)
C2F	928(2)	-35(2)	-1318.4(18)	8.8(5)
C5C	6462(2)	6753(2)	7635.3(19)	14.0(6)
C7E	3972(2)	4195(2)	763.9(19)	11.5(6)

O81E	1844.3(15)	2118.8(14)	-1625.1(13)	10.6(4)
C7C	5321(2)	7574(2)	5628.0(18)	9.9(5)
C6C	6976(2)	7017(2)	7119.3(18)	10.6(6)
C8C	8007(2)	7051(2)	7211.6(18)	10.4(6)
C6F	437(2)	1124(2)	-438.7(18)	7.9(5)
C2E	3504(2)	4430(2)	31.0(18)	9.9(5)
C8F	763(2)	2110(2)	196.4(18)	8.3(5)
N1A	6972.3(17)	7245.2(17)	4051.9(15)	8.5(5)
C2B	9181(2)	9905(2)	6715.6(18)	9.2(5)
C8A	6763(2)	5688(2)	4150.1(19)	14.6(6)
C6D	4261(2)	1137(2)	697.9(18)	10.2(6)
C3B	10004(2)	10636(2)	6998.9(19)	13.3(6)
N1E	2909.0(17)	3667.3(17)	-566.7(15)	7.6(5)
C6E	2454(2)	3768(2)	-1259.1(18)	8.4(5)
C4C	5510(2)	6753(2)	7492(2)	17.6(7)
C4B	10819(2)	10446(2)	6780(2)	16.4(6)
C8D	3332(2)	938(2)	931.0(18)	11.1(6)
C3D	5848(2)	1583(2)	165(2)	16.0(6)
C7B	8256(2)	9998(2)	6920.1(17)	8.4(5)
C7F	1767(2)	-269(2)	-1623.1(19)	10.5(6)
C2D	4991(2)	1724(2)	-176.6(18)	9.6(5)
C3A	6457(2)	7588(2)	2821.3(18)	10.2(6)
C5A	6166(2)	5970(2)	2801.6(19)	13.9(6)
C4A	6074(2)	6622(2)	2395.1(18)	13.0(6)
O1	5000.4(16)	8900.2(16)	2863.9(14)	14.5(4)
O2	4158.5(16)	392.1(17)	2936.7(14)	15.8(5)
O3	3820.4(17)	-99.5(16)	-2265.6(14)	17.1(5)
O4	2596.7(16)	7225.7(16)	1268.2(14)	16.3(5)
O5	-2198.7(16)	1512.8(17)	-415.8(15)	18.1(5)
O6	-2946.1(18)	3627.2(18)	2438.7(16)	23.8(5)
O7	2875(2)	7983.4(18)	7007.0(16)	25.6(6)
O8	3241(2)	5745(2)	2181.2(18)	38.3(7)
O9	-902(4)	6116(2)	3485.7(18)	75.2(16)
O10	4325(4)	5397(3)	4588(4)	94.2(19)
O11A	2460(5)	5290(5)	4414(4)	47(2)
O11B	1751(4)	5191(4)	4651(4)	23.2(17)
O12	-629(5)	3948(5)	4368(4)	133(3)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Nd-III. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U2	5.18(4)	4.46(4)	6.39(4)	2.61(3)	0.40(3)	0.68(3)
U1	6.35(4)	4.51(4)	5.31(4)	1.83(3)	-1.27(3)	0.26(3)
Nd2	5.32(7)	7.80(7)	7.09(7)	0.18(6)	-0.60(5)	1.33(5)
Nd1	6.43(7)	4.06(7)	6.66(7)	2.57(5)	-1.26(5)	0.79(5)
O72A	13.9(11)	8.6(10)	14.3(11)	7.1(8)	4.8(8)	2.8(8)

O72F	21.2(12)	6.8(10)	21.1(12)	2.2(9)	12.9(10)	2.6(9)
O82E	15.9(11)	14.9(11)	11(1)	6.3(9)	-2.7(9)	3.1(9)
O82C	15.7(11)	18.1(11)	11.3(10)	9.0(9)	0.6(9)	9.2(9)
O4W	10.7(10)	9.4(10)	16.1(11)	4.3(9)	3.2(9)	0.6(8)
O72B	13.5(11)	8.8(10)	17.7(11)	1.2(9)	5.4(9)	3.5(8)
O71G	12.1(10)	6.1(9)	10.5(10)	3.6(8)	-2.1(8)	0.9(8)
O81G	15.2(11)	7.6(10)	10.4(10)	1.4(8)	-4.7(8)	2.0(8)
O10W	18.0(12)	13.3(11)	12.0(11)	2.9(9)	1.2(9)	5.2(9)
O72D	9.6(10)	16.6(11)	13.6(11)	4.7(9)	6.6(8)	1.0(8)
O71D	9(1)	13.8(10)	10(1)	6.5(8)	3.1(8)	3.1(8)
O1W	10.5(10)	7.2(9)	9.3(10)	1.8(8)	0.0(8)	1.5(8)
O82F	9.1(10)	8.7(10)	12(1)	1.1(8)	2.9(8)	2.8(8)
O11W	11.9(11)	10.5(10)	25.1(13)	1.7(9)	8.7(9)	2.0(9)
O6W	10.8(10)	18.5(11)	11.7(10)	3.0(9)	1.8(8)	2.9(9)
O82A	39.0(16)	9.8(11)	17.0(12)	2.6(9)	0.2(11)	2.1(10)
O00Q	9.8(10)	18.9(11)	12.8(10)	9.8(9)	3.5(8)	6.5(9)
O72G	9.6(10)	10.2(10)	7.8(10)	4.1(8)	-2.7(8)	1.0(8)
O82B	18.0(12)	11.5(11)	32.7(14)	-1.1(10)	15.7(11)	1.1(9)
O9W	11.6(10)	12.9(10)	8.4(10)	3.4(8)	-0.1(8)	2.0(8)
O82G	14.1(11)	8.4(10)	13.4(11)	-0.4(8)	-7.0(9)	-1.7(8)
O71E	12.8(10)	8.7(10)	8.3(10)	3.5(8)	-0.4(8)	0.1(8)
N1C	8.9(12)	7.2(11)	7.2(11)	3.2(9)	-1.4(9)	1.5(9)
C2G	5.9(12)	8.1(13)	7.7(13)	3(1)	2.7(10)	2.8(10)
O7W	17.3(12)	15.0(11)	16.0(11)	3.8(9)	1.3(9)	-1.9(9)
C4G	10.7(14)	6.8(13)	14.4(14)	4.6(11)	3.3(11)	3.2(11)
O2W	14.7(12)	27.2(13)	26.0(13)	19.8(11)	0.9(10)	4.4(10)
C3G	9.5(13)	7.9(13)	11.2(14)	4.1(11)	0.4(11)	3.1(11)
O72C	9.4(10)	18.0(11)	13.6(11)	8.5(9)	1.0(8)	4.6(9)
O81D	9(1)	15.1(11)	15.1(11)	10.0(9)	3.8(8)	3.5(8)
O71A	13.5(10)	7.2(10)	8.6(10)	2.7(8)	-0.9(8)	0.4(8)
O72E	19.8(12)	11.4(11)	14.1(11)	-0.1(9)	-6.2(9)	-4.1(9)
C5G	8.1(13)	6.0(13)	13.5(14)	0.8(11)	0.7(11)	0.1(10)
O82D	17.6(12)	23.9(12)	19.6(12)	17.7(10)	4.7(9)	4.6(10)
O5W	31.0(15)	30.3(15)	20.4(13)	-10.5(11)	-9.2(11)	21.2(12)
N1D	8.9(12)	7.2(11)	9.1(11)	2.4(9)	1.5(9)	2.6(9)
C2A	6.3(13)	9.5(13)	7.5(13)	3.2(11)	1(1)	1.5(10)
N1B	9.4(12)	6.4(11)	7.5(11)	1.3(9)	0.8(9)	1.3(9)
C5B	9.3(14)	16.8(15)	14.2(15)	0.5(12)	3.7(12)	0.7(12)
C5E	13.2(14)	11.0(14)	15.0(15)	6.2(12)	2.5(12)	3.9(11)
O81C	11.4(10)	15.3(11)	10.9(10)	8.1(9)	0.7(8)	3.4(8)
C6G	5.2(12)	7.3(13)	9.8(13)	1.5(11)	0.6(10)	1.6(10)
O71B	7.5(10)	7.8(10)	10.2(10)	1.4(8)	1.1(8)	-0.3(8)
O3W	16.0(11)	8.2(10)	15.4(11)	1.8(9)	5.4(9)	3.0(8)
O81B	11.2(10)	8.7(10)	13.2(10)	-0.6(8)	3.9(8)	0.0(8)
N1F	8.2(11)	7.3(11)	8.1(11)	4.2(9)	1.7(9)	3.0(9)
C4D	13.5(16)	30.2(19)	19.5(17)	12.4(15)	2.1(13)	12.5(14)
C7G	5.3(12)	7.7(13)	7.8(13)	2.9(10)	2(1)	1.6(10)
C8E	7.5(13)	9.8(13)	10.0(13)	2.2(11)	1.4(11)	1.9(11)

C4F	7.7(13)	10.5(14)	14.4(14)	3.1(12)	0.1(11)	-2.4(11)
C5D	16.6(16)	19.2(16)	14.5(15)	9.6(13)	1.3(12)	8.2(13)
O71C	8.5(10)	13.7(10)	10.8(10)	7.4(8)	0.0(8)	1.5(8)
C7A	2.9(12)	10.4(13)	11.2(13)	4.6(11)	3.3(10)	2.1(10)
O81F	8.6(10)	6.6(9)	12.1(10)	2.7(8)	2.7(8)	1.3(8)
O81A	20.1(12)	8.5(10)	9.7(10)	3.5(8)	-2.2(9)	-1.1(9)
C2C	11.6(14)	8.8(13)	9.9(13)	5.6(11)	-0.7(11)	1.8(11)
C5F	8.3(13)	11.4(14)	12.6(14)	4.9(11)	2.1(11)	2.8(11)
C6A	11.1(14)	8.2(13)	11.6(14)	3.1(11)	1.0(11)	1.0(11)
C4E	19.0(16)	8.8(14)	22.2(17)	7.6(13)	5.3(13)	3.7(12)
C3C	13.4(15)	18.1(16)	16.1(15)	9.5(13)	4.6(12)	4.3(12)
C3E	14.0(15)	7.0(13)	16.8(15)	2.0(12)	1.0(12)	-0.8(11)
C8G	9.5(13)	9.7(13)	9.7(13)	1.9(11)	0.0(11)	3.1(11)
O71F	10.3(10)	7.3(10)	14.8(11)	2.7(8)	4.1(8)	1.6(8)
C3F	13.1(14)	6.2(13)	12.4(14)	1.1(11)	2.4(11)	-0.1(11)
C7D	10.7(14)	5.9(12)	7.6(13)	0.1(10)	1.2(11)	1.4(10)
C6B	9.9(14)	10.0(13)	9.1(13)	1.7(11)	1.8(11)	1.8(11)
N1G	6.0(11)	6.8(11)	7.3(11)	2.3(9)	-0.5(9)	1.6(9)
C8B	13.3(14)	9.4(14)	10.8(14)	1.3(11)	4.7(11)	1.3(11)
C2F	11.5(14)	6.3(13)	8.9(13)	3.5(11)	2.0(11)	2.0(11)
C5C	16.1(15)	16.2(15)	12.1(14)	10.0(12)	1.4(12)	3.7(12)
C7E	10.8(14)	12.1(14)	11.7(14)	4.4(12)	3.0(11)	2.4(11)
O81E	13(1)	5.9(9)	10.1(10)	2.8(8)	-1.9(8)	0.3(8)
C7C	12.6(14)	7.2(13)	8.9(13)	1.9(11)	0.7(11)	3.3(11)
C6C	11.4(14)	10.0(13)	9.1(13)	3.7(11)	-0.8(11)	2.7(11)
C8C	13.9(14)	6.8(13)	8.7(13)	2.2(11)	-1.0(11)	2.8(11)
C6F	7.5(13)	7.6(13)	8.8(13)	3.8(11)	-0.2(10)	3(1)
C2E	8.3(13)	9.7(13)	10.6(14)	2.7(11)	2.2(11)	1.2(11)
C8F	9.0(13)	7.1(13)	9.0(13)	4.1(11)	-0.8(10)	3.1(10)
N1A	8.0(11)	8.6(11)	7.7(11)	3.1(9)	0.0(9)	0.7(9)
C2B	11.4(14)	6.8(13)	8.4(13)	1.8(11)	1.0(11)	2.2(11)
C8A	16.7(15)	10.9(14)	12.7(15)	4.0(12)	-0.7(12)	-0.5(12)
C6D	10.6(14)	10.0(13)	11.1(14)	4.8(11)	2.2(11)	3.8(11)
C3B	13.7(15)	7.9(13)	13.0(14)	-2.2(11)	3.4(12)	-0.2(11)
N1E	6.5(11)	6.6(11)	9.3(11)	2.6(9)	1.7(9)	1.0(9)
C6E	6.6(13)	9.8(13)	9.3(13)	3.8(11)	1.5(10)	3.1(10)
C4C	17.7(16)	22.3(17)	17.7(16)	13.4(14)	6.0(13)	4.7(13)
C4B	10.2(14)	14.8(15)	14.6(15)	-4.1(12)	2.9(12)	-4.8(12)
C8D	11.9(14)	11.7(14)	9.6(13)	4.8(11)	1.2(11)	2.1(11)
C3D	11.3(15)	21.3(16)	17.6(16)	7.0(13)	5.3(12)	6.8(12)
C7B	8.2(13)	9.6(13)	6.4(13)	3.0(11)	-1.1(10)	2.2(10)
C7F	12.8(14)	8.4(13)	12.2(14)	5.5(11)	3.9(11)	2.8(11)
C2D	10.5(14)	8.0(13)	10.6(13)	3.0(11)	3.7(11)	2.2(11)
C3A	10.0(14)	13.6(14)	8.5(13)	5.3(11)	2.5(11)	3.5(11)
C5A	15.0(15)	10.6(14)	10.2(14)	0.0(11)	-1.7(12)	-0.2(12)
C4A	11.8(14)	17.2(15)	6.4(13)	1.5(12)	0.2(11)	1.5(12)
O1	13.2(11)	17.0(11)	13.4(11)	5.8(9)	3.5(9)	3.0(9)
O2	14.3(11)	19.9(12)	15.2(11)	7.9(9)	3.8(9)	6.0(9)

O3	20.8(12)	16.8(11)	18.4(12)	8.5(10)	8.5(10)	8.9(9)
O4	13.7(11)	15.7(11)	14.2(11)	0.2(9)	2.1(9)	0.3(9)
O5	14.3(11)	19.5(12)	21.0(12)	7(1)	4.0(9)	5.6(9)
O6	23.3(13)	23.1(13)	28.3(14)	8.0(11)	14.8(11)	6.8(11)
O7	33.9(15)	21.2(13)	18.3(13)	6.2(10)	8.7(11)	-1.8(11)
O8	28.9(16)	41.5(18)	23.6(15)	-9.8(13)	-3.2(12)	2.5(13)
O9	184(5)	24.1(16)	11.1(14)	-1.1(12)	-6(2)	53(2)
O10	72(3)	47(2)	153(5)	45(3)	-17(3)	17(2)
O12	198(7)	172(6)	187(6)	155(6)	173(6)	147(6)

Table 4 Bond Lengths for U-Nd-III.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U2	O71D	2.369(2)		O71A	C7A	1.289(4)
U2	O71E	2.349(2)		O72E	C7E	1.227(4)
U2	O81D	2.372(2)		C5G	C6G	1.386(4)
U2	N1D	2.553(2)		O82D	C8D	1.233(4)
U2	N1F	2.556(2)		N1D	C6D	1.343(4)
U2	O81F	2.419(2)		N1D	C2D	1.339(4)
U2	O71F	2.398(2)		C2A	C7A	1.504(4)
U2	O81E	2.330(2)		C2A	N1A	1.341(4)
U2	N1E	2.571(2)		C2A	C3A	1.389(4)
U1	N1C	2.530(2)		N1B	C6B	1.340(4)
U1	O71A	2.413(2)		N1B	C2B	1.341(4)
U1	N1B	2.519(2)		C5B	C6B	1.383(4)
U1	O81C	2.407(2)		C5B	C4B	1.389(4)
U1	O71B	2.350(2)		C5E	C4E	1.393(4)
U1	O81B	2.374(2)		C5E	C6E	1.388(4)
U1	O71C	2.414(2)		O81C	C8C	1.288(4)
U1	O81A	2.336(2)		C6G	C8G	1.514(4)
U1	N1A	2.525(2)		C6G	N1G	1.339(4)
Nd2	O10W	2.503(2)		O71B	C7B	1.302(4)
Nd2	O11W	2.497(2)		O81B	C8B	1.278(4)
Nd2	O6W	2.522(2)		N1F	C2F	1.340(4)
Nd2	O00Q	2.571(2)		N1F	C6F	1.337(4)
Nd2	O9W	2.603(2)		C4D	C5D	1.392(5)
Nd2	O82G	2.433(2)		C4D	C3D	1.395(5)
Nd2	O7W	2.460(2)		C8E	O81E	1.293(4)
Nd2	O72C	2.524(2)		C8E	C6E	1.511(4)
Nd2	O5W	2.432(2)		C4F	C5F	1.392(4)
Nd1	O82C[1]	2.535(2)		C4F	C3F	1.397(4)
Nd1	O4W	2.487(2)		C5D	C6D	1.384(4)
Nd1	O71G	2.437(2)		O71C	C7C	1.285(4)
Nd1	O81G	2.489(2)		O81F	C8F	1.288(4)
Nd1	O1W	2.587(2)		O81A	C8A	1.305(4)
Nd1	O82F	2.540(2)		C2C	C3C	1.387(4)
Nd1	O2W	2.495(2)		C2C	C7C	1.507(4)

Nd1	O3W	2.466(2)		C5F	C6F	1.385(4)
Nd1	N1G	2.549(2)		C6A	N1A	1.339(4)
O72A	C7A	1.237(3)		C6A	C8A	1.507(4)
O72F	C7F	1.234(4)		C6A	C5A	1.384(4)
O82E	C8E	1.227(4)		C4E	C3E	1.394(5)
O82C	Nd1[1]	2.535(2)		C3C	C4C	1.394(4)
O82C	C8C	1.243(4)		C3E	C2E	1.384(4)
O72B	C7B	1.221(4)		O71F	C7F	1.286(4)
O71G	C7G	1.262(3)		C3F	C2F	1.395(4)
O81G	C8G	1.268(4)		C7D	C2D	1.512(4)
O72D	C7D	1.239(4)		C6B	C8B	1.511(4)
O71D	C7D	1.285(4)		C2F	C7F	1.510(4)
O82F	C8F	1.237(4)		C5C	C6C	1.385(4)
O82A	C8A	1.226(4)		C5C	C4C	1.393(5)
O72G	C7G	1.254(3)		C7E	C2E	1.513(4)
O82B	C8B	1.236(4)		C6C	C8C	1.502(4)
O82G	C8G	1.247(4)		C6F	C8F	1.509(4)
O71E	C7E	1.287(4)		C2E	N1E	1.338(4)
N1C	C2C	1.340(4)		C2B	C3B	1.386(4)
N1C	C6C	1.345(4)		C2B	C7B	1.510(4)
C2G	C3G	1.391(4)		C6D	C8D	1.515(4)
C2G	C7G	1.517(4)		C3B	C4B	1.395(4)
C2G	N1G	1.345(4)		N1E	C6E	1.341(4)
C4G	C3G	1.393(4)		C3D	C2D	1.388(4)
C4G	C5G	1.395(4)		C3A	C4A	1.388(4)
O72C	C7C	1.236(4)		C5A	C4A	1.387(4)
O81D	C8D	1.287(4)		O11A	O11B	1.206(8)

[1]1-X,1-Y,1-Z

II.18 U-Nd-IV

Table 1 Crystal data and structure refinement for U-Nd-IV.	
Identification code	U-Nd-IV
Empirical formula	$C_{28}H_{24}N_4NdO_{28}U$
Formula weight	1246.78
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	12.0918(12)
b/Å	12.9459(12)
c/Å	14.7053(15)
α/°	109.669(4)
β/°	105.488(5)
γ/°	100.170(4)

Volume/Å^3	1996.9(3)
Z	2
ρ_{calc}g/cm^3	2.074
μ/mm^{-1}	5.441
F(000)	1192.0
Crystal size/mm^3	0.15 × 0.137 × 0.101
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.142 to 60.858
Index ranges	-16 ≤ h ≤ 17, -18 ≤ k ≤ 16, -20 ≤ l ≤ 20
Reflections collected	51444
Independent reflections	11921 [R_{int} = 0.0332, R_{sigma} = 0.0375]
Data/restraints/parameters	11921/0/535
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0301, wR_2 = 0.0716
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.0758
Largest diff. peak/hole / e Å^{-3}	1.55/-0.99

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Nd-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	2564.3(2)	3261.6(2)	6252.4(2)	19.19(4)
Nd1	1259.6(2)	7432.5(2)	9803.0(2)	21.45(5)
O81B	2748(2)	5279(2)	7210(2)	27.2(5)
O71B	3945(2)	2592(2)	5553(2)	28.2(6)
O81D	1393(2)	3143(2)	7315(2)	28.2(6)
O71D	2009(2)	3696(2)	4778(2)	29.0(6)
O71A	2099(3)	6407(2)	10898.7(19)	29.4(6)
N1B	4394(2)	4778(2)	6471(2)	18.4(5)
N1D	470(3)	3472(2)	5677(2)	21.3(6)
O3W	-650(3)	7394(3)	8583(2)	38.5(7)
N1A	2353(3)	8596(2)	11779(2)	24.1(6)
O81A	1422(3)	9462(2)	10477(2)	34.8(6)
O2W	3466(3)	8263(3)	10228(2)	43.2(7)
O81C	1290(2)	1515(2)	4926(2)	31.8(6)
O1W	-268(3)	7470(3)	10654(2)	40.0(7)
O5W	1917(3)	5847(2)	8818(3)	44.4(8)
O4W	-225(3)	5482(2)	9113(3)	45.3(8)
O82D	-189(3)	3288(2)	7810(2)	33.5(6)
O72B	5585(2)	2742(2)	5124(2)	30.9(6)
O71C	3987(2)	3530(2)	7888(2)	29.3(6)
N1C	2748(3)	1465(2)	6537(2)	25.5(6)
O82B	3544(3)	7168(2)	7742(2)	38.4(7)
C2D	49(3)	3559(3)	4782(3)	21.3(7)
C7A	2689(3)	6881(3)	11827(3)	26.1(8)
C7B	4918(3)	3154(3)	5531(3)	21.6(7)
C6B	4537(3)	5905(3)	6947(3)	21.3(7)
C2B	5207(3)	4440(3)	6072(2)	18.8(6)
C6D	-244(3)	3413(3)	6229(3)	21.5(7)

C7D	952(3)	3627(3)	4243(3)	26.4(7)
O72D	642(3)	3628(3)	3381(2)	48.2(8)
C3D	-1115(3)	3585(3)	4387(3)	27.5(8)
C8D	349(3)	3272(3)	7202(3)	25.3(7)
O6W	1679(3)	7857(3)	8371(2)	48.1(8)
C8B	3554(3)	6168(3)	7340(3)	24.9(7)
C2A	2868(3)	8124(3)	12399(3)	24.7(7)
O72A	3163(3)	6357(2)	12366(2)	38.0(7)
O82C	621(3)	-394(3)	4115(2)	50.1(9)
C4D	-1854(4)	3531(3)	4955(3)	30.1(8)
C5B	5508(3)	6737(3)	7049(3)	28.6(8)
O82A	1763(4)	11141(2)	11767(3)	61.8(11)
C5D	-1408(3)	3452(3)	5898(3)	28.4(8)
C8A	1828(4)	10151(3)	11423(3)	32.0(9)
C3B	6210(3)	5229(3)	6156(3)	26.8(8)
O72C	5024(3)	2912(3)	8978(3)	58.3(10)
C6A	2433(4)	9707(3)	12184(3)	28.2(8)
C6C	2094(4)	451(3)	5790(3)	36.0(9)
C7C	4264(4)	2740(3)	8151(3)	32.5(9)
C5A	3033(4)	10383(3)	13229(3)	37.2(10)
C8C	1251(4)	493(3)	4855(3)	32.1(9)
C4B	6352(3)	6384(3)	6639(3)	28.6(8)
C2C	3563(4)	1532(3)	7388(3)	36.1(9)
C3A	3494(4)	8744(3)	13440(3)	35.9(9)
O1S	3487(4)	4885(4)	9693(3)	75.1(12)
C4A	3571(4)	9894(3)	13856(3)	41.3(11)
C3C	3748(6)	563(4)	7525(5)	73(2)
C5C	2217(6)	-555(4)	5881(5)	74(2)
O6S	241(6)	9156(5)	7290(5)	119(2)
C4C	3046(7)	-494(4)	6753(6)	100(3)
O3S	8566(5)	9152(4)	10699(4)	86.8(14)
O4S	6417(12)	7867(12)	9682(10)	271(6)
O5S	5520(6)	9382(6)	9096(5)	131(2)
O2S	-2796(4)	5705(3)	8819(3)	62.9(10)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Nd-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	16.29(7)	20.36(6)	20.36(7)	7.64(5)	6.69(5)	4.89(5)
Nd1	25.38(10)	22.57(8)	17.02(9)	8.18(7)	6.27(8)	10.03(7)
O81B	25.1(14)	26.4(12)	31.5(14)	8.6(10)	15.3(11)	8.4(10)
O71B	24.2(13)	21.1(11)	36.8(15)	6.4(10)	15.1(12)	4.6(10)
O81D	24.9(14)	37.9(14)	28.4(14)	18.6(11)	12.1(11)	10.1(11)
O71D	22.1(13)	43.9(15)	29.1(14)	20.9(12)	12.7(11)	10.3(11)
O71A	40.4(16)	25.1(12)	20.3(13)	8(1)	5.0(11)	15.0(11)
N1B	14.7(13)	19.8(12)	21.2(14)	8.1(10)	7.0(11)	5.1(10)

N1D	19.1(14)	25.0(13)	21.4(14)	9.6(11)	9.0(12)	7.1(11)
O3W	38.7(17)	58.3(18)	28.8(15)	22.5(14)	12.6(13)	27.6(15)
N1A	28.5(17)	21.7(13)	20.5(14)	8.2(11)	4.9(12)	9.6(12)
O81A	50.0(18)	28.6(13)	26.0(14)	13.7(11)	6.0(13)	18.2(13)
O2W	32.0(17)	55.4(18)	46.5(19)	26.4(16)	11.8(14)	14.5(14)
O81C	27.9(14)	28.2(12)	27.3(14)	7.2(11)	0.7(11)	1.9(11)
O1W	47.5(19)	54.9(18)	31.3(16)	22.0(14)	22.0(14)	25.4(15)
O5W	58(2)	39.1(15)	48.9(19)	15.4(14)	36.0(17)	21.6(15)
O4W	41.3(18)	33.1(14)	59(2)	10.9(14)	25.5(16)	8.3(13)
O82D	37.5(16)	42.2(15)	32.6(15)	20.8(12)	22.2(13)	12.8(13)
O72B	28.9(15)	30.6(13)	37.0(15)	10.2(11)	18.5(12)	13.4(11)
O71C	28.2(14)	23.6(11)	26.9(13)	6.3(10)	0.7(11)	7.4(10)
N1C	25.9(16)	21.6(13)	24.6(15)	8.1(11)	5.9(13)	4.0(12)
O82B	36.0(16)	25.5(12)	54.6(19)	9.6(12)	23.3(14)	13.3(12)
C2D	17.9(17)	25.4(15)	19.0(16)	7.3(13)	6.1(13)	6.5(13)
C7A	29(2)	24.8(16)	23.6(18)	11.0(14)	4.8(15)	11.6(15)
C7B	22.2(18)	23.0(15)	20.2(16)	8.3(13)	7.3(14)	8.9(13)
C6B	19.9(17)	24.0(15)	20.6(16)	8.7(13)	7.3(14)	8.1(13)
C2B	18.2(16)	22.4(14)	17.9(15)	9.2(12)	7.1(13)	7.0(12)
C6D	19.3(17)	23.1(15)	22.8(17)	9.0(13)	9.9(14)	4.1(13)
C7D	26.0(19)	33.1(18)	21.6(18)	11.6(14)	9.0(15)	10.2(15)
O72D	41.8(19)	88(3)	23.8(15)	27.3(16)	15.2(14)	26.3(18)
C3D	24.1(19)	30.1(17)	24.9(18)	8.3(14)	5.2(15)	11.0(15)
C8D	27.2(19)	23.0(15)	27.5(19)	10.9(14)	13.3(16)	5.0(14)
O6W	48(2)	84(2)	35.0(17)	38.7(17)	20.1(15)	33.5(18)
C8B	20.0(18)	25.9(16)	26.7(18)	8.5(14)	7.9(15)	6.7(14)
C2A	29(2)	25.1(16)	19.0(16)	8.9(13)	5.1(15)	11.5(14)
O72A	52.3(19)	31.8(14)	29.5(15)	15.3(12)	4.2(13)	20.9(13)
O82C	50(2)	33.2(15)	36.5(17)	-2.6(13)	-0.5(15)	-1.4(14)
C4D	23.0(19)	34.0(18)	37(2)	14.9(16)	12.4(17)	14.6(16)
C5B	30(2)	20.7(15)	34(2)	8.9(14)	13.3(17)	5.9(14)
O82A	92(3)	26.7(14)	44.7(19)	7.3(13)	-8.5(19)	29.2(17)
C5D	23.2(19)	31.2(17)	35(2)	11.8(15)	17.0(16)	10.6(15)
C8A	37(2)	24.4(16)	31(2)	9.9(15)	6.7(17)	11.5(16)
C3B	22.7(18)	30.7(17)	29.8(19)	11.3(15)	14.3(16)	8.4(15)
O72C	62(2)	41.8(17)	43.5(19)	11.4(15)	-16.9(17)	16.4(16)
C6A	34(2)	22.4(15)	24.7(18)	9.0(14)	3.8(16)	11.2(15)
C6C	40(2)	22.4(16)	35(2)	8.4(15)	4.7(18)	3.2(16)
C7C	29(2)	29.7(18)	30(2)	8.3(15)	1.6(17)	8.2(16)
C5A	50(3)	22.6(16)	28(2)	4.5(15)	4.8(19)	10.8(17)
C8C	28(2)	28.3(17)	29(2)	4.4(15)	8.1(17)	0.7(15)
C4B	23.2(19)	27.6(17)	33(2)	12.3(15)	10.9(16)	2.0(14)
C2C	35(2)	25.7(17)	38(2)	11.8(16)	0.9(18)	6.8(16)
C3A	45(3)	32.4(19)	25(2)	11.8(16)	1.9(18)	13.2(18)
C4A	55(3)	30.1(19)	19.9(19)	1.6(15)	-3.2(18)	9.7(19)
C3C	90(5)	33(2)	65(4)	21(2)	-20(3)	13(3)
C5C	85(4)	19.9(19)	73(4)	10(2)	-17(3)	1(2)
C4C	121(6)	26(2)	97(5)	25(3)	-34(5)	7(3)

Table 4 Bond Lengths for U-Nd-IV.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
U1	O81B	2.451(2)		O71C	C7C	1.275(5)
U1	O71B	2.329(2)		N1C	C6C	1.324(5)
U1	O81D	2.395(3)		N1C	C2C	1.335(5)
U1	O71D	2.376(3)		O82B	C8B	1.233(4)
U1	N1B	2.552(3)		C2D	C7D	1.518(5)
U1	N1D	2.540(3)		C2D	C3D	1.383(5)
U1	O81C	2.342(3)		C7A	C2A	1.488(5)
U1	O71C	2.425(3)		C7A	O72A	1.294(4)
U1	N1C	2.535(3)		C7B	C2B	1.510(4)
Nd1	O71A	2.536(2)		C6B	C8B	1.498(5)
Nd1	O3W	2.498(3)		C6B	C5B	1.383(5)
Nd1	N1A	2.600(3)		C2B	C3B	1.389(5)
Nd1	O81A	2.425(3)		C6D	C8D	1.507(5)
Nd1	O2W	2.512(3)		C6D	C5D	1.377(5)
Nd1	O1W	2.491(3)		C7D	O72D	1.223(5)
Nd1	O5W	2.476(3)		C3D	C4D	1.385(6)
Nd1	O4W	2.516(3)		C2A	C3A	1.379(5)
Nd1	O6W	2.498(3)		O82C	C8C	1.221(5)
O81B	C8B	1.290(4)		C4D	C5D	1.392(6)
O71B	C7B	1.284(4)		C5B	C4B	1.386(5)
O81D	C8D	1.276(4)		O82A	C8A	1.235(4)
O71D	C7D	1.279(5)		C8A	C6A	1.505(5)
O71A	C7A	1.229(4)		C3B	C4B	1.377(5)
N1B	C6B	1.344(4)		O72C	C7C	1.233(5)
N1B	C2B	1.337(4)		C6A	C5A	1.389(5)
N1D	C2D	1.329(4)		C6C	C8C	1.502(6)
N1D	C6D	1.343(4)		C6C	C5C	1.381(6)
N1A	C2A	1.342(4)		C7C	C2C	1.506(5)
N1A	C6A	1.332(4)		C5A	C4A	1.375(6)
O81A	C8A	1.271(5)		C2C	C3C	1.381(6)
O81C	C8C	1.283(5)		C3A	C4A	1.381(5)
O82D	C8D	1.234(4)		C3C	C4C	1.382(7)
O72B	C7B	1.220(4)		C5C	C4C	1.369(8)

II.19 U-Sm-IV

Table 1 Crystal data and structure refinement for U-Sm-IV.	
Identification code	U-Sm-IV
Empirical formula	$C_{28}H_{24}N_4O_{28}SmU$
Formula weight	1252.91
Temperature/K	296.15

Crystal system	triclinic
Space group	P-1
a/Å	12.1116(10)
b/Å	12.9089(11)
c/Å	14.6970(13)
α/°	109.818(4)
β/°	105.438(4)
γ/°	99.937(4)
Volume/Å^3	1994.3(3)
Z	2
ρ_{calc}g/cm^3	2.0862
μ/mm^{-1}	5.620
F(000)	1176.7
Crystal size/mm^3	N/A × N/A × N/A
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.14 to 61.66
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 18, -21 ≤ l ≤ 21
Reflections collected	117032
Independent reflections	12461 [R_{int} = 0.0437, R_{sigma} = 0.0244]
Data/restraints/parameters	12461/0/534
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0253, wR_2 = 0.0709
Final R indexes [all data]	R_1 = 0.0295, wR_2 = 0.0733
Largest diff. peak/hole / e Å^{-3}	3.38/-1.33

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Sm-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	2569.39(9)	3259.03(9)	6239.43(8)	18.40(3)
Sm1	1270.79(13)	7425.58(13)	9815.52(11)	21.98(4)
O81B	2742(2)	5273.3(19)	7203.2(19)	26.7(5)
O71B	3949(2)	2589.1(19)	5537(2)	29.4(5)
O81D	1406(2)	3141(2)	7308.2(18)	28.0(5)
O71D	2011(2)	3690(2)	4764.8(18)	28.4(5)
O71A	2073(2)	6393(2)	10891.3(18)	30.7(5)
N1B	4389(2)	4783(2)	6467.3(19)	19.4(4)
N1D	476(2)	3468(2)	5671.3(19)	20.6(5)
O3W	-618(2)	7399(3)	8611(2)	38.4(6)
N1A	2343(2)	8586(2)	11768(2)	25.2(5)
O81A	1419(3)	9435(2)	10457.1(19)	34.0(5)
O2W	3445(2)	8241(2)	10231(2)	40.3(6)
O81C	1297(2)	1509(2)	4917.2(19)	32.0(5)
O1W	-236(3)	7472(3)	10654(2)	38.7(6)
O5W	1927(3)	5855(2)	8833(3)	47.1(7)
O4W	-202(3)	5498(2)	9114(3)	46.4(7)
O82D	-169(2)	3289(2)	7809(2)	33.8(5)
O72B	5596(2)	2741(2)	5120(2)	32.6(5)
O71C	4001(2)	3532(2)	7867.9(18)	29.5(5)

N1C	2765(2)	1464(2)	6530(2)	26.1(5)
O82B	3526(2)	7169(2)	7739(2)	36.3(6)
C2D	54(3)	3561(3)	4775(2)	21.1(5)
C7A	2662(3)	6864(3)	11821(2)	26.1(6)
C7B	4925(3)	3157(3)	5522(2)	22.1(5)
C6B	4528(3)	5906(3)	6944(2)	21.2(5)
C2B	5205(2)	4442(2)	6072(2)	19.7(5)
C6D	-230(3)	3413(3)	6224(2)	21.6(5)
C7D	949(3)	3624(3)	4235(2)	26.4(6)
O72D	635(3)	3621(3)	3370(2)	47.7(8)
C3D	-1111(3)	3589(3)	4380(3)	27.3(6)
C8D	362(3)	3268(3)	7195(2)	24.7(6)
O6W	1667(3)	7836(3)	8393(2)	47.9(8)
C8B	3539(3)	6168(3)	7340(2)	23.9(6)
C2A	2851(3)	8112(3)	12390(2)	25.1(6)
O72A	3131(3)	6338(2)	12362(2)	39.6(6)
O82C	615(3)	-403(2)	4112(2)	50.3(8)
C4D	-1847(3)	3531(3)	4957(3)	29.1(7)
C5B	5502(3)	6744(3)	7055(3)	28.5(6)
O82A	1755(4)	11132(2)	11736(3)	61.4(10)
C5D	-1399(3)	3452(3)	5898(3)	28.0(6)
C8A	1815(3)	10138(3)	11400(3)	32.3(7)
C3B	6209(3)	5233(3)	6164(3)	26.8(6)
O72C	5053(3)	2914(3)	8951(3)	64.5(11)
C6A	2423(3)	9697(3)	12170(3)	29.4(7)
C6C	2097(4)	443(3)	5791(3)	36.4(8)
C7C	4281(3)	2745(3)	8136(3)	33.5(7)
C5A	3025(4)	10387(3)	13215(3)	38.8(9)
C8C	1254(3)	485(3)	4853(3)	31.7(7)
C4B	6355(3)	6389(3)	6654(3)	29.5(7)
C2C	3581(4)	1534(3)	7377(3)	37.5(8)
C3A	3478(4)	8743(3)	13440(3)	35.5(8)
O1S	3474(5)	4879(4)	9678(4)	90.8(14)
C4A	3564(4)	9897(3)	13848(3)	41.5(9)
C3C	3756(6)	571(4)	7519(5)	76(2)
C5C	2213(6)	-563(4)	5884(5)	78(2)
O6S	235(6)	9137(5)	7278(5)	115.4(19)
C4C	3038(7)	-500(4)	6753(6)	109(3)
O3S	8618(4)	9175(4)	10719(4)	81.2(12)
O4S	6388(10)	7906(10)	9724(9)	221(4)
O5S	5489(6)	9409(5)	9055(5)	112.5(18)
O2S	-2738(4)	5734(4)	8827(3)	70.6(11)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Sm-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}

U1	15.76(5)	19.02(5)	19.54(5)	4.53(4)	6.05(4)	7.14(4)
Sm1	26.19(7)	22.99(7)	17.20(7)	9.87(6)	6.58(5)	8.13(6)
O81B	25.3(10)	24.3(11)	32.1(12)	7.6(8)	15.5(9)	9.0(9)
O71B	26.4(11)	20.5(10)	39.0(13)	5.3(8)	16.5(10)	6.3(9)
O81D	25.3(10)	38.1(13)	26.9(11)	10.5(9)	11.9(9)	17.9(10)
O71D	22.3(10)	43.3(14)	27.8(11)	10.4(9)	13.1(9)	20.4(10)
O71A	43.3(13)	24.8(11)	21.2(11)	16(1)	5.5(10)	7.7(9)
N1B	17.4(10)	19.6(11)	21.9(11)	6.1(8)	8.1(9)	7.8(9)
N1D	17.8(10)	24.1(12)	19.8(11)	5.5(9)	7.4(9)	8.4(9)
O3W	41.1(14)	55.7(17)	27.1(12)	27.0(13)	10.8(11)	21.5(12)
N1A	31.7(13)	20.8(12)	20.9(12)	10(1)	5.9(10)	7.2(10)
O81A	48.8(15)	25.8(12)	27.1(12)	16.0(11)	7.0(11)	12.7(10)
O2W	31.0(13)	46.6(16)	44.7(16)	12.7(11)	11.0(11)	21.2(13)
O81C	30.7(12)	27.5(12)	27.3(12)	3.0(9)	2.6(9)	7.4(10)
O1W	44.8(15)	53.1(17)	31.6(13)	23.8(13)	21.4(12)	22.1(12)
O5W	63.0(19)	38.1(15)	52.1(18)	20.6(14)	39.6(16)	14.4(13)
O4W	41.9(15)	33.8(14)	60.4(19)	7.1(12)	23.8(14)	13.0(13)
O82D	37.7(13)	44.0(14)	30.8(12)	13.0(11)	22.2(11)	19.8(11)
O72B	31.2(12)	30.2(12)	40.8(14)	14.5(10)	20.8(11)	10.5(11)
O71C	28.2(11)	22.3(11)	27.9(11)	7.1(9)	0.0(9)	6.1(9)
N1C	26.7(12)	20.6(12)	26.0(13)	4.6(10)	5.5(10)	7.6(10)
O82B	37.0(13)	24.1(11)	49.4(16)	13.2(10)	22.3(12)	9.1(11)
C2D	20.7(12)	23.2(13)	19.0(13)	7.5(10)	7.7(10)	7.1(11)
C7A	32.2(15)	24.6(14)	22.2(14)	13.4(12)	6.5(12)	10.0(12)
C7B	20.4(12)	22.9(13)	22.1(13)	7.4(10)	7.1(10)	7.7(11)
C6B	20.9(12)	21.7(13)	22.4(13)	7.5(10)	8.7(10)	9.1(11)
C2B	17.8(11)	21.6(13)	20.9(13)	6.9(10)	7.4(10)	8.9(11)
C6D	21.5(12)	22.0(13)	22.1(13)	5.8(10)	10.4(10)	8.3(11)
C7D	25.7(14)	34.2(16)	21.0(14)	9.6(12)	9.7(11)	11.4(12)
O72D	43.5(15)	85(2)	23.0(12)	25.2(16)	15.3(11)	26.5(14)
C3D	24.6(14)	30.9(16)	24.5(15)	11.2(12)	6.6(11)	9.1(12)
C8D	27.0(14)	23.8(14)	25.1(14)	5.8(11)	12.0(12)	10.7(12)
O6W	47.5(16)	81(2)	36.2(15)	32.5(16)	21.0(13)	37.0(16)
C8B	21.8(13)	25.3(14)	25.4(14)	9.5(11)	9.2(11)	9.2(12)
C2A	29.7(14)	23.1(14)	20.8(14)	10.5(12)	5.4(11)	8.1(11)
O72A	57.2(17)	32.9(13)	27.6(12)	22.8(12)	3.9(11)	14.8(11)
O82C	51.5(17)	31.8(14)	37.4(15)	-2.1(12)	-0.8(13)	-1.7(12)
C4D	21.8(13)	32.2(16)	34.0(17)	12.3(12)	9.9(12)	11.9(14)
C5B	28.9(15)	21.2(14)	34.7(17)	5.9(12)	14.6(13)	8.7(13)
O82A	89(3)	26.0(14)	45.6(18)	27.9(15)	-8.5(16)	5.8(12)
C5D	23.8(14)	30.6(16)	32.5(16)	9.1(12)	15.5(12)	11.1(13)
C8A	38.5(18)	23.4(15)	31.4(17)	10.9(13)	6.1(14)	10.5(13)
C3B	23.2(13)	28.0(15)	33.3(16)	8.6(12)	15.9(12)	12.0(13)
O72C	69(2)	37.0(16)	49.8(19)	14.6(15)	-25.6(16)	9.4(14)
C6A	35.3(16)	22.1(14)	26.6(15)	11.3(12)	5.2(13)	8.0(12)
C6C	39.9(19)	18.9(15)	36.4(19)	1.7(13)	4.3(15)	5.1(13)
C7C	31.1(16)	27.2(16)	31.1(17)	8.2(13)	-1.4(13)	8.5(13)
C5A	53(2)	23.7(16)	29.2(17)	13.3(15)	5.0(16)	4.1(13)

C8C	28.7(15)	27.1(16)	28.4(16)	1.4(12)	7.5(13)	3.8(13)
C4B	24.4(14)	27.5(15)	36.3(18)	2.6(12)	14.2(13)	12.3(14)
C2C	40.0(19)	25.4(16)	38.0(19)	7.9(14)	0.5(15)	13.0(15)
C3A	43.8(19)	31.8(17)	23.6(16)	13.2(15)	1.6(14)	9.4(14)
C4A	56(2)	29.5(18)	21.5(16)	9.8(16)	-2.2(15)	3.2(13)
C3C	92(4)	32(2)	69(3)	11(2)	-23(3)	22(2)
C5C	95(4)	19.7(19)	73(4)	3(2)	-21(3)	11(2)
C4C	137(7)	25(2)	98(5)	7(3)	-45(5)	23(3)

Table 4 Bond Lengths for U-Sm-IV.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O81B	2.443(2)		O71C	C7C	1.273(4)
U1	O71B	2.328(2)		N1C	C6C	1.329(4)
U1	O81D	2.396(2)		N1C	C2C	1.332(4)
U1	O71D	2.373(2)		O82B	C8B	1.230(4)
U1	N1B	2.551(2)		C2D	C7D	1.512(4)
U1	N1D	2.542(2)		C2D	C3D	1.388(4)
U1	O81C	2.341(2)		C7A	C2A	1.485(4)
U1	O71C	2.422(2)		C7A	O72A	1.294(4)
U1	N1C	2.532(3)		C7B	C2B	1.507(4)
Sm1	O71A	2.506(2)		C6B	C8B	1.505(4)
Sm1	O3W	2.479(2)		C6B	C5B	1.387(4)
Sm1	N1A	2.568(3)		C2B	C3B	1.390(4)
Sm1	O81A	2.396(2)		C6D	C8D	1.506(4)
Sm1	O2W	2.483(3)		C6D	C5D	1.384(4)
Sm1	O1W	2.457(3)		C7D	O72D	1.224(4)
Sm1	O5W	2.451(3)		C3D	C4D	1.393(5)
Sm1	O4W	2.488(3)		C2A	C3A	1.390(4)
Sm1	O6W	2.466(3)		O82C	C8C	1.223(4)
O81B	C8B	1.289(4)		C4D	C5D	1.391(5)
O71B	C7B	1.288(4)		C5B	C4B	1.389(5)
O81D	C8D	1.277(4)		O82A	C8A	1.232(4)
O71D	C7D	1.285(4)		C8A	C6A	1.511(5)
O71A	C7A	1.230(4)		C3B	C4B	1.374(5)
N1B	C6B	1.336(4)		O72C	C7C	1.230(4)
N1B	C2B	1.338(4)		C6A	C5A	1.391(5)
N1D	C2D	1.334(4)		C6C	C8C	1.505(5)
N1D	C6D	1.336(4)		C6C	C5C	1.377(6)
N1A	C2A	1.341(4)		C7C	C2C	1.505(5)
N1A	C6A	1.328(4)		C5A	C4A	1.382(5)
O81A	C8A	1.271(4)		C2C	C3C	1.370(6)
O81C	C8C	1.284(4)		C3A	C4A	1.378(5)
O82D	C8D	1.236(4)		C3C	C4C	1.394(7)
O72B	C7B	1.220(4)		C5C	C4C	1.364(8)

II.20 U-Eu-IV

Table 1 Crystal data and structure refinement for U-Eu-IV.	
Identification code	U-Eu-IV
Empirical formula	$C_{28}H_{24}EuN_4O_{28}U$
Formula weight	1254.50
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	12.0871(4)
b/Å	12.9180(5)
c/Å	14.6723(6)
α/°	109.831(2)
β/°	105.550(2)
γ/°	99.973(2)
Volume/Å^3	1986.07(13)
Z	2
ρ_{calc}g/cm^3	2.098
μ/mm^{-1}	5.743
F(000)	1198.0
Crystal size/mm^3	0.186 × 0.139 × 0.121
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.154 to 61.068
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	68114
Independent reflections	11998 [R_{int} = 0.0293, R_{sigma} = 0.0221]
Data/restraints/parameters	11998/0/535
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0237, wR_2 = 0.0625
Final R indexes [all data]	R_1 = 0.0283, wR_2 = 0.0647
Largest diff. peak/hole / e Å^{-3}	1.61/-0.97

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Eu-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	7565.9(2)	3262.3(2)	6251.4(2)	18.40(3)
Eu1	3741.5(2)	2572.2(2)	10180.7(2)	21.00(4)
O82A	4810(2)	3299(2)	7814.3(19)	33.8(5)
O81D	2925(2)	3603.6(19)	9114.2(17)	29.2(5)
O71A	7015.1(18)	3693(2)	4774.5(17)	28.0(5)
O81C	7740.5(19)	5280.8(18)	7215.9(17)	26.6(4)
O71C	8950.6(19)	2590.9(18)	5551.0(18)	28.3(5)
O81B	8994(2)	3532.2(18)	7891.4(17)	28.4(5)
O82C	8538(2)	7176(2)	7763(2)	36.9(6)
O72C	10590(2)	2742(2)	5117.6(19)	32.5(5)

O81A	6393.0(19)	3148(2)	7316.4(17)	28.2(5)
O72A	5647(2)	3623(3)	3372(2)	48.1(7)
O1W	1572(2)	1770(2)	9784(2)	40.8(6)
O6W	5616(2)	2598(2)	11377(2)	39.9(6)
O2W	5221(2)	2514(3)	9323(2)	38.8(6)
O71B	6291(2)	1512(2)	4919.6(18)	32.0(5)
N1C	9394(2)	4783(2)	6481.4(18)	19.0(4)
O82D	1858(2)	3661(2)	7648.6(19)	37.9(6)
O71D	3599(2)	572(2)	9548.5(18)	34.0(5)
N1D	2664(2)	1414(2)	8233.3(19)	25.0(5)
O5W	3340(3)	2155(3)	11596(2)	47.3(7)
O3W	5208(2)	4487(2)	10859(2)	44.5(6)
N1B	7757(2)	1465(2)	6539(2)	25.6(5)
N1A	5469(2)	3476(2)	5671.9(18)	20.4(4)
C2C	10208(2)	4447(2)	6080(2)	19.5(5)
O72B	5611(3)	-401(2)	4109(2)	50.0(7)
O82B	10038(3)	2913(3)	8980(2)	58.7(9)
O4W	3081(3)	4126(2)	11159(2)	44.1(6)
O72D	3257(3)	-1127(2)	8269(2)	60.3(10)
C4A	3141(3)	3531(3)	4947(3)	29.7(6)
C6C	9538(2)	5911(2)	6962(2)	21.5(5)
C7C	9928(2)	3158(3)	5531(2)	22.5(5)
C5C	10511(3)	6743(3)	7069(3)	27.1(6)
C4C	11362(3)	6391(3)	6657(3)	29.3(6)
C3C	11215(3)	5235(3)	6171(3)	26.3(6)
C5A	3586(3)	3460(3)	5889(3)	27.7(6)
C3A	3885(3)	3585(3)	4371(2)	26.2(6)
C8C	8546(3)	6172(3)	7354(2)	24.0(6)
C2A	5054(2)	3562(2)	4775(2)	21.6(5)
C6A	4762(2)	3422(2)	6227(2)	21.9(5)
C8A	5350(3)	3278(3)	7199(2)	24.4(6)
C6D	2145(3)	1884(3)	7609(2)	24.9(6)
C7A	5957(3)	3626(3)	4240(2)	26.1(6)
C8D	2333(3)	3135(3)	8182(2)	25.7(6)
C2D	2582(3)	301(3)	7831(2)	28.8(6)
C6B	8578(3)	1532(3)	7391(3)	36.1(8)
C7D	3195(3)	-131(3)	8602(3)	33.6(7)
C2B	7091(3)	443(3)	5793(3)	36.1(7)
C8B	9268(3)	2739(3)	8154(3)	32.0(7)
C4D	1432(4)	99(3)	6147(3)	41.2(9)
C3D	1983(4)	-388(3)	6783(3)	38.4(8)
C7B	6245(3)	486(3)	4849(3)	32.1(7)
C5D	1518(3)	1258(3)	6559(3)	35.5(7)
C5B	8751(5)	568(4)	7530(4)	72.9(18)
C4B	8035(6)	-504(4)	6750(5)	104(3)
C3B	7207(5)	-566(4)	5884(4)	76.9(19)
O1S	2224(3)	5724(3)	8848(3)	65.4(9)
O2S	1517(3)	5108(3)	10317(3)	70.5(10)

O3S	6406(4)	834(4)	9289(4)	88.4(13)
O4S	4769(5)	862(5)	2720(5)	116.4(18)
O6S	523(6)	-602(5)	9098(5)	121.8(19)
O5S	8567(10)	2140(10)	10288(8)	233(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U-Eu-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	15.91(5)	19.29(5)	19.09(5)	6.91(4)	6.30(4)	4.64(3)
Eu1	25.26(7)	21.91(7)	16.28(7)	7.61(5)	6.23(5)	9.98(5)
O82A	37.7(12)	43.6(14)	31.6(12)	19.6(11)	22.8(10)	13.6(10)
O81D	40.3(12)	23.8(10)	20(1)	6.7(9)	4.9(9)	14.3(9)
O71A	20.9(9)	43.8(13)	26.8(11)	20.2(10)	11.8(8)	10.0(9)
O81C	25.4(10)	24.6(10)	30.4(11)	8.2(9)	14.5(9)	7.4(8)
O71C	25.9(10)	20.7(10)	37.0(13)	6.6(9)	16.3(9)	6.1(8)
O81B	28.1(10)	21.5(10)	27.3(11)	6.3(9)	1.7(9)	7.5(8)
O82C	37.7(13)	24.4(11)	50.6(16)	8.8(11)	24.3(12)	12.9(10)
O72C	31.2(11)	30.2(12)	39.1(13)	9.6(10)	20.1(10)	13.5(9)
O81A	26.2(10)	38.6(12)	26.4(11)	18.1(10)	12.2(9)	10.4(9)
O72A	41.3(14)	88(2)	24.3(13)	26.9(14)	15.3(11)	25.6(15)
O1W	29.8(12)	45.8(15)	46.8(16)	22.1(13)	9.0(11)	11.1(11)
O6W	42.8(14)	56.8(17)	28.8(13)	21.5(12)	11.7(11)	28.6(13)
O2W	44.4(14)	49.5(15)	33.8(13)	20.3(12)	21.4(11)	21.3(12)
O71B	30.1(11)	27.9(11)	27.6(12)	8.2(9)	2.4(9)	2.2(9)
N1C	17.3(10)	19.1(11)	21.5(11)	7.6(9)	8.0(9)	6.6(8)
O82D	53.6(15)	31.1(12)	27.0(12)	13.8(10)	3.5(11)	20.8(11)
O71D	49.4(14)	27.3(11)	24.7(11)	12.7(9)	6.4(10)	16(1)
N1D	31.4(13)	21.0(12)	20.2(12)	7.1(10)	5.4(10)	10.2(10)
O5W	48.9(16)	78(2)	34.3(14)	33.6(15)	20.6(12)	34.1(15)
O3W	37.6(13)	33.2(13)	55.8(18)	8.8(12)	20.5(13)	6.9(11)
N1B	26.1(12)	19.9(11)	25.9(13)	7.1(10)	5.8(10)	4.7(9)
N1A	18.6(10)	22.9(11)	19.7(11)	8.0(9)	7.9(9)	5.6(8)
C2C	18.7(11)	20.5(12)	20.5(13)	8.8(10)	7.4(10)	7.3(10)
O72B	51.5(17)	31.2(14)	35.8(15)	-3.2(11)	-1.0(12)	-2.8(12)
O82B	60.0(19)	38.6(15)	46.8(17)	11.9(13)	-20.3(14)	13.8(14)
O4W	61.4(17)	35.6(14)	46.2(16)	13.8(12)	36.3(14)	18.7(13)
O72D	88(2)	25.8(13)	45.2(17)	6.4(12)	-7.2(16)	27.9(15)
C4A	22.2(13)	33.9(16)	32.7(17)	11.3(14)	9.3(12)	12.4(12)
C6C	21.0(12)	20.9(13)	22.2(13)	7.7(11)	8.1(10)	6.7(10)
C7C	21.3(12)	24.7(14)	22.4(14)	10.1(11)	7.4(10)	8(1)
C5C	28.0(14)	19.0(13)	32.3(16)	7.7(12)	12.6(12)	4.2(11)
C4C	25.1(14)	25.6(15)	35.2(17)	10.7(13)	13.3(13)	1.7(11)
C3C	21.6(13)	27.3(14)	32.8(16)	10.6(13)	15.2(12)	8.2(11)
C5A	22.2(13)	30.7(15)	33.1(16)	11.2(13)	15.3(12)	9.7(11)
C3A	24.2(13)	30.1(15)	22.1(14)	8.1(12)	5.6(11)	11.4(11)
C8C	24.8(13)	22.6(13)	23.7(14)	6.5(11)	9.8(11)	9.0(11)

C2A	20.9(12)	23.5(13)	18.8(13)	7.3(11)	6.2(10)	6.3(10)
C6A	22.1(12)	21.6(13)	22.9(14)	7.5(11)	11.5(11)	6.1(10)
C8A	26.8(13)	25.4(14)	23.9(14)	10.8(12)	12.9(11)	6.9(11)
C6D	31.2(14)	22.5(14)	19.4(13)	7.7(11)	6.2(11)	9.8(11)
C7A	27.1(14)	33.1(16)	19.6(14)	10.1(12)	10.3(11)	10.3(12)
C8D	31.7(15)	25.2(14)	20.0(14)	9.3(11)	6.3(11)	12.3(12)
C2D	34.7(16)	21.6(14)	25.3(15)	6.7(12)	5.2(12)	10.8(12)
C6B	38.8(18)	23.8(15)	35.9(18)	11.1(14)	0.8(14)	7.5(13)
C7D	41.8(18)	22.7(15)	32.0(17)	9.8(13)	5.6(14)	13.7(13)
C2B	38.3(17)	22.2(15)	36.1(19)	7.5(14)	5.0(14)	2.1(13)
C8B	29.1(15)	27.3(15)	32.3(17)	10.3(13)	1.5(13)	9.3(12)
C4D	55(2)	29.0(17)	21.1(16)	1.8(13)	-2.5(15)	10.7(16)
C3D	53(2)	21.9(15)	27.1(17)	2.7(13)	3.0(15)	11.8(14)
C7B	29.7(15)	28.8(16)	27.2(16)	4.8(13)	6.7(13)	2.2(12)
C5D	44.9(19)	29.1(16)	25.1(16)	9.6(13)	1.4(14)	12.8(14)
C5B	86(4)	32(2)	66(3)	20(2)	-22(3)	10(2)
C4B	128(6)	27(2)	99(5)	25(3)	-38(4)	8(3)
C3B	89(4)	22.0(19)	73(3)	11(2)	-23(3)	1(2)

Table 4 Bond Lengths for U-Eu-IV.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O71A	2.371(2)		N1D	C6D	1.342(4)
U1	O81C	2.448(2)		N1D	C2D	1.330(4)
U1	O71C	2.330(2)		N1B	C6B	1.337(4)
U1	O81B	2.426(2)		N1B	C2B	1.330(4)
U1	O81A	2.397(2)		N1A	C2A	1.326(4)
U1	O71B	2.342(2)		N1A	C6A	1.338(3)
U1	N1C	2.550(2)		C2C	C7C	1.511(4)
U1	N1B	2.534(3)		C2C	C3C	1.388(4)
U1	N1A	2.543(2)		O72B	C7B	1.219(4)
Eu1	O81D	2.498(2)		O82B	C8B	1.235(4)
Eu1	O1W	2.474(2)		O72D	C7D	1.235(4)
Eu1	O6W	2.453(2)		C4A	C5A	1.383(5)
Eu1	O2W	2.445(2)		C4A	C3A	1.397(4)
Eu1	O71D	2.388(2)		C6C	C5C	1.383(4)
Eu1	N1D	2.555(3)		C6C	C8C	1.504(4)
Eu1	O5W	2.459(3)		C5C	C4C	1.392(4)
Eu1	O3W	2.473(3)		C4C	C3C	1.374(4)
Eu1	O4W	2.438(3)		C5A	C6A	1.390(4)
O82A	C8A	1.244(4)		C3A	C2A	1.388(4)
O81D	C8D	1.230(4)		C2A	C7A	1.513(4)
O71A	C7A	1.279(4)		C6A	C8A	1.502(4)
O81C	C8C	1.289(4)		C6D	C8D	1.490(4)
O71C	C7C	1.291(3)		C6D	C5D	1.385(4)
O81B	C8B	1.275(4)		C2D	C7D	1.504(4)
O82C	C8C	1.234(4)		C2D	C3D	1.390(5)

O72C	C7C	1.219(4)		C6B	C8B	1.498(5)
O81A	C8A	1.275(4)		C6B	C5B	1.369(5)
O72A	C7A	1.226(4)		C2B	C7B	1.510(5)
O71B	C7B	1.284(4)		C2B	C3B	1.381(6)
N1C	C2C	1.337(3)		C4D	C3D	1.385(5)
N1C	C6C	1.341(4)		C4D	C5D	1.385(5)
O82D	C8D	1.288(4)		C5B	C4B	1.398(7)
O71D	C7D	1.273(4)		C4B	C3B	1.357(7)

II.21 U-Gd-IV

Table 1 Crystal data and structure refinement for U-Gd-IV.	
Identification code	U-Gd-IV
Empirical formula	$C_{28}H_{24}GdN_4O_{28}U$
Formula weight	1259.79
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	12.1006(11)
b/Å	12.9368(10)
c/Å	14.6826(13)
α/°	109.972(4)
β/°	105.437(4)
γ/°	99.959(4)
Volume/Å^3	1992.0(3)
Z	2
ρ_{calc}g/cm^3	2.100
μ/mm^{-1}	5.816
F(000)	1200.0
Crystal size/mm^3	0.265 × 0.189 × 0.134
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.152 to 60.988
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	66788
Independent reflections	12042 [R_{int} = 0.0293, R_{sigma} = 0.0211]
Data/restraints/parameters	12042/0/535
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0243, wR_2 = 0.0680
Final R indexes [all data]	R_1 = 0.0273, wR_2 = 0.0696
Largest diff. peak/hole / e Å^{-3}	3.01/-1.20

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Gd-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
U1	2569.6(2)	3263.8(2)	6241.6(2)	18.72(3)

Gd1	1270.0(2)	7426.3(2)	9821.2(2)	20.91(4)
O81B	2742(2)	5279.4(19)	7211.0(18)	26.2(4)
O71B	3947(2)	2587.4(18)	5536.4(19)	28.5(5)
O81D	1403(2)	3147(2)	7312.0(18)	27.6(5)
O71D	2012.5(19)	3690(2)	4763.3(18)	28.1(5)
O71A	2064(2)	6388.5(19)	10883.9(17)	29.8(5)
N1B	4393(2)	4787(2)	6472.1(19)	19.2(4)
N1D	474(2)	3473(2)	5669.2(19)	20.4(4)
O3W	-598(2)	7405(2)	8630(2)	37.2(6)
N1A	2334(2)	8580(2)	11761(2)	24.5(5)
O81A	1406(2)	9421(2)	10442.9(18)	32.9(5)
O2W	3424(2)	8232(2)	10233(2)	39.0(6)
O81C	1295(2)	1508(2)	4912.0(19)	31.6(5)
O1W	-218(3)	7476(3)	10660(2)	38.1(6)
O5W	1918(3)	5870(2)	8843(2)	45.2(7)
O4W	-197(3)	5519(2)	9124(3)	45.0(7)
O82D	-178(2)	3300(2)	7812(2)	33.8(5)
O72B	5596(2)	2741(2)	5119(2)	32.5(5)
O71C	4002(2)	3535.2(19)	7874.6(18)	29.0(5)
N1C	2767(2)	1469(2)	6533(2)	26.1(5)
O82B	3532(2)	7177(2)	7755(2)	36.0(6)
C2D	53(3)	3560(2)	4767(2)	21.0(5)
C7A	2653(3)	6861(3)	11815(2)	25.3(6)
C7B	4925(3)	3156(3)	5523(2)	22.1(5)
C6B	4533(3)	5913(2)	6956(2)	21.1(5)
C2B	5209(2)	4447(2)	6077(2)	19.9(5)
C6D	-230(3)	3422(2)	6224(2)	21.5(5)
C7D	954(3)	3624(3)	4231(2)	26.3(6)
O72D	638(3)	3619(3)	3363(2)	48.7(8)
C3D	-1113(3)	3589(3)	4372(3)	26.9(6)
C8D	360(3)	3278(3)	7196(2)	23.8(6)
O6W	1661(3)	7837(3)	8409(2)	46.4(7)
C8B	3544(3)	6174(3)	7351(2)	23.5(6)
C2A	2848(3)	8113(3)	12387(2)	25.8(6)
O72A	3124(3)	6332(2)	12355(2)	38.5(6)
O82C	610(3)	-405(2)	4109(2)	50.4(8)
C4D	-1850(3)	3534(3)	4949(3)	28.7(6)
C5B	5504(3)	6748(3)	7065(3)	28.2(6)
O82A	1742(3)	11124(2)	11716(2)	60.1(10)
C5D	-1400(3)	3460(3)	5893(3)	27.2(6)
C8A	1803(3)	10127(3)	11383(3)	32.2(7)
C3B	6213(3)	5233(3)	6172(3)	26.2(6)
O72C	5059(3)	2915(3)	8958(3)	63.9(11)
C6A	2413(3)	9696(3)	12162(3)	28.1(6)
C6C	2099(3)	444(3)	5790(3)	36.3(8)
C7C	4285(3)	2746(3)	8137(3)	34.0(7)
C5A	3017(4)	10388(3)	13207(3)	38.9(8)
C8C	1252(3)	485(3)	4853(3)	32.2(7)

C4B	6359(3)	6392(3)	6662(3)	29.1(6)
C2C	3585(3)	1535(3)	7376(3)	37.0(8)
C3A	3474(3)	8742(3)	13437(3)	34.9(7)
O1S	3473(4)	4886(4)	9679(4)	86.6(13)
C4A	3559(4)	9901(3)	13845(3)	40.8(9)
C3C	3765(6)	572(4)	7519(5)	78(2)
C5C	2214(6)	-561(4)	5883(5)	78(2)
O6S	236(6)	9141(6)	7283(5)	120(2)
C4C	3039(7)	-503(4)	6755(5)	107(3)
O3S	8628(4)	9176(4)	10724(4)	80.3(12)
O4S	6409(10)	7895(10)	9726(9)	217(4)
O5S	5494(6)	9421(5)	9081(5)	112.1(18)
O2S	-2731(4)	5739(4)	8839(3)	68.6(10)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Gd-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	15.77(5)	19.60(5)	19.59(6)	7.11(4)	6.06(4)	4.40(4)
Gd1	24.81(7)	22.18(7)	15.93(7)	7.62(5)	6.07(5)	9.31(5)
O81B	23.4(10)	25(1)	30.5(12)	8.1(9)	14.2(9)	7.0(8)
O71B	25.0(11)	19.7(10)	38.4(13)	5.6(9)	16.3(10)	5.3(8)
O81D	25.6(11)	36.7(12)	24.3(11)	16(1)	10.2(9)	9.1(9)
O71D	20.6(10)	44.1(13)	26.3(11)	20.3(10)	10.8(9)	9.2(9)
O71A	42.1(13)	23(1)	20.1(11)	6.4(9)	4.7(10)	14.3(10)
N1B	17(1)	19.6(11)	20.2(11)	6.9(9)	7.0(9)	5.5(8)
N1D	19.1(11)	23.5(11)	18.5(11)	7.8(9)	8.0(9)	5.0(9)
O3W	40.7(14)	51.5(15)	27.7(13)	20.0(12)	11.6(11)	25.8(12)
N1A	29.8(13)	21.0(11)	20.3(12)	6.9(10)	5.5(10)	9.7(10)
O81A	47.4(15)	26.5(11)	23.8(11)	11.1(9)	7.2(10)	15.3(10)
O2W	30.8(13)	45.5(15)	43.2(15)	21.5(13)	11.0(11)	13.5(11)
O81C	29.3(12)	27.3(11)	26.8(12)	7.3(9)	2.0(9)	1.3(9)
O1W	44.9(15)	51.1(16)	29.2(13)	20.0(12)	19.8(12)	21.8(13)
O5W	62.8(19)	36.7(14)	48.4(17)	14.0(13)	38.6(15)	20.3(13)
O4W	39.9(15)	33.4(13)	56.1(18)	11.1(13)	21.3(14)	5.5(11)
O82D	37.0(13)	43.9(14)	31.1(13)	19.8(11)	22.1(11)	12.4(11)
O72B	30.7(12)	29.7(12)	39.6(14)	8.9(10)	20.1(11)	12.9(10)
O71C	28.4(11)	22.4(10)	26.9(12)	6.4(9)	0.6(9)	6.6(9)
N1C	26.0(13)	20.1(11)	26.2(13)	6.8(10)	5.1(10)	4.1(10)
O82B	36.5(13)	23.7(11)	48.8(16)	8.8(11)	22.0(12)	12.7(10)
C2D	19.0(12)	23.7(13)	18.6(13)	6.9(11)	6.2(10)	6(1)
C7A	31.5(15)	23.3(13)	21.1(14)	9.4(11)	6.5(12)	12.2(12)
C7B	20.3(13)	22.5(13)	22.3(14)	7.7(11)	7.1(11)	7(1)
C6B	19.7(13)	20.9(12)	22.1(14)	7.2(11)	8.1(11)	6.8(10)
C2B	18.2(12)	21.6(12)	19.9(13)	8(1)	6.5(10)	7.1(10)
C6D	20.3(13)	22.4(13)	21.2(13)	7.6(11)	9.0(11)	4.8(10)
C7D	26.9(15)	33.7(16)	20.7(14)	11.5(12)	10.7(12)	9.8(12)

O72D	41.7(16)	90(2)	23.9(13)	27.9(15)	15.8(12)	25.4(16)
C3D	22.8(14)	30.7(15)	23.4(15)	8.2(12)	4.9(12)	10.1(12)
C8D	25.3(14)	24.7(13)	22.6(14)	9.6(11)	11.0(12)	6.1(11)
O6W	46.7(16)	80(2)	32.5(14)	34.5(15)	20.0(13)	32.8(16)
C8B	22.3(13)	22.2(13)	25.5(15)	7.4(11)	9.7(11)	8.7(11)
C2A	31.3(15)	24.4(14)	21.0(14)	9.6(11)	6.2(12)	10.5(12)
O72A	55.7(17)	30.5(12)	26.5(12)	12.8(10)	3.0(11)	21.3(12)
O82C	51.4(18)	30.9(14)	37.4(16)	-2.9(12)	-1.3(13)	-2.5(12)
C4D	21.5(14)	32.9(16)	31.0(17)	10.5(13)	8.2(12)	12.9(12)
C5B	28.7(15)	21.8(13)	32.8(17)	8.9(12)	13.2(13)	4.9(12)
O82A	86(2)	25.7(13)	45.4(17)	6.9(12)	-8.1(16)	27.2(15)
C5D	21.8(14)	28.6(15)	32.1(16)	9.7(13)	14.3(12)	7.7(11)
C8A	39.7(18)	22.1(14)	31.3(17)	11.0(13)	5.5(14)	11.5(13)
C3B	20.6(13)	28.4(14)	32.3(16)	11.2(13)	14.7(12)	7.4(11)
O72C	67(2)	38.3(16)	49.1(19)	10.3(14)	-25.6(16)	14.9(15)
C6A	33.7(16)	21.2(13)	25.5(15)	7.9(12)	5.6(13)	9.6(12)
C6C	37.7(19)	19.8(14)	37.1(19)	7.4(13)	2.1(15)	0.7(13)
C7C	33.1(17)	26.8(15)	32.8(18)	10.1(14)	-0.3(14)	9.2(13)
C5A	52(2)	23.7(15)	28.1(18)	3.7(13)	3.9(16)	12.1(15)
C8C	29.3(16)	27.1(15)	28.3(17)	3.4(13)	7.1(13)	1.0(12)
C4B	25.0(15)	25.1(14)	35.1(18)	10.7(13)	13.7(13)	0.9(12)
C2C	37.8(19)	24.8(15)	37.6(19)	12.0(14)	-1.2(15)	7.3(13)
C3A	42.6(19)	31.6(17)	23.1(16)	9.5(13)	1.3(14)	12.7(15)
C4A	56(2)	28.1(16)	20.4(16)	1.6(13)	-1.8(15)	9.6(16)
C3C	92(4)	32(2)	73(4)	22(2)	-25(3)	12(2)
C5C	91(4)	20.1(18)	73(4)	11(2)	-24(3)	0(2)
C4C	130(6)	24(2)	98(5)	21(3)	-46(4)	5(3)

Table 4 Bond Lengths for U-Gd-IV.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O81B	2.447(2)		O71C	C7C	1.275(4)
U1	O71B	2.328(2)		N1C	C6C	1.332(4)
U1	O81D	2.399(2)		N1C	C2C	1.329(4)
U1	O71D	2.374(2)		O82B	C8B	1.232(4)
U1	N1B	2.551(2)		C2D	C7D	1.511(4)
U1	N1D	2.543(2)		C2D	C3D	1.388(4)
U1	O81C	2.347(2)		C7A	C2A	1.489(4)
U1	O71C	2.425(2)		C7A	O72A	1.298(4)
U1	N1C	2.540(3)		C7B	C2B	1.515(4)
Gd1	O71A	2.498(2)		C6B	C8B	1.502(4)
Gd1	O3W	2.451(2)		C6B	C5B	1.385(4)
Gd1	N1A	2.545(3)		C2B	C3B	1.384(4)
Gd1	O81A	2.384(2)		C6D	C8D	1.506(4)
Gd1	O2W	2.456(3)		C6D	C5D	1.385(4)
Gd1	O1W	2.434(3)		C7D	O72D	1.227(4)
Gd1	O5W	2.429(3)		C3D	C4D	1.393(5)

Gd1	O4W	2.465(3)		C2A	C3A	1.387(5)
Gd1	O6W	2.448(3)		O82C	C8C	1.226(4)
O81B	C8B	1.291(4)		C4D	C5D	1.390(5)
O71B	C7B	1.290(4)		C5B	C4B	1.392(5)
O81D	C8D	1.276(4)		O82A	C8A	1.236(4)
O71D	C7D	1.281(4)		C8A	C6A	1.514(4)
O71A	C7A	1.229(4)		C3B	C4B	1.378(4)
N1B	C6B	1.341(4)		O72C	C7C	1.236(4)
N1B	C2B	1.336(4)		C6A	C5A	1.389(5)
N1D	C2D	1.338(4)		C6C	C8C	1.505(5)
N1D	C6D	1.334(4)		C6C	C5C	1.380(5)
N1A	C2A	1.342(4)		C7C	C2C	1.504(5)
N1A	C6A	1.335(4)		C5A	C4A	1.387(5)
O81A	C8A	1.267(4)		C2C	C3C	1.375(5)
O81C	C8C	1.286(4)		C3A	C4A	1.384(5)
O82D	C8D	1.243(4)		C3C	C4C	1.396(7)
O72B	C7B	1.220(4)		C5C	C4C	1.367(7)

II.22 U-Tb-IV

Table 1 Crystal data and structure refinement for U-Tb-IV.	
Identification code	U-Tb-IV
Empirical formula	$C_{28}H_{24}N_4O_{29}TbU$
Formula weight	1277.46
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	12.1326(9)
b/Å	12.8001(9)
c/Å	14.5777(11)
α/°	109.908(3)
β/°	105.717(3)
γ/°	99.782(3)
Volume/Å^3	1961.2(3)
Z	2
ρ_{calc}g/cm^3	2.163
μ/mm^{-1}	6.023
F(000)	1218.0
Crystal size/mm^3	0.383 × 0.346 × 0.158
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.178 to 61.036
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
Reflections collected	75572
Independent reflections	11935 [R_{int} = 0.0242, R_{sigma} = 0.0142]
Data/restraints/parameters	11935/0/539

Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0263, wR_2 = 0.0677
Final R indexes [all data]	R_1 = 0.0267, wR_2 = 0.0680
Largest diff. peak/hole / e $Å^{-3}$	5.57/-1.91

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Tb-IV. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	7433.4(2)	6721.8(2)	3795.2(2)	6.21(3)
Tb1	1309.4(2)	7417.5(2)	-170.2(2)	7.10(3)
O72B	4410(2)	7265(2)	4905.3(19)	12.8(4)
O81A	1417(2)	9427(2)	438.4(18)	12.1(4)
O1W	-178(2)	7498(2)	640.9(18)	12.9(4)
O82A	1666(3)	11117(2)	1738(2)	22.1(6)
O3W	-566(2)	7356(2)	-1394.3(18)	13.1(4)
O71A	2033(3)	6355(2)	887.8(19)	18.5(5)
O82B	6458(2)	2767(2)	2252.5(19)	11.6(4)
O81B	7235(2)	4682.5(19)	2789.4(18)	9.7(4)
O81D	8569(2)	6839(2)	2692.1(18)	10.1(4)
O72D	9387(2)	6255(3)	6637(2)	19.9(5)
O71B	6072(2)	7404.6(19)	4500.5(19)	11.3(4)
O71D	8016(2)	6285(2)	5270.7(18)	10.4(4)
O4W	-124(2)	5498(2)	-862(2)	19.8(5)
O82D	10149(2)	6715(2)	2184.6(18)	11.7(4)
N1C	7241(2)	8522(2)	3485(2)	10.4(5)
O82C	9445(2)	10430(2)	5902.8(19)	16.9(5)
O72A	3069(3)	6280(2)	2379.4(19)	19.0(5)
N1A	2330(2)	8569(2)	1775(2)	9.3(4)
O5W	1990(3)	5883(2)	-1117(2)	21.4(5)
O81C	8726(2)	8487(2)	5118.9(18)	12.0(4)
O3AA	5966(2)	6432(2)	2154.3(18)	11.9(4)
O6W	1690(2)	7858(3)	-1559(2)	19.9(5)
O2W	3433(2)	8229(2)	256.2(19)	13.2(4)
N1D	9528(2)	6506(2)	4343(2)	7.4(4)
N1B	5604(2)	5188(2)	3547(2)	7.4(4)
C6D	10231(3)	6588(3)	3788(2)	8.0(5)
C6A	2399(3)	9694(3)	2180(2)	10.9(5)
C7B	5076(3)	6833(3)	4498(2)	9.3(5)
C6B	5449(3)	4049(3)	3047(2)	7.7(5)
C8D	9617(3)	6731(3)	2806(2)	9.2(5)
C4D	11875(3)	6499(3)	5073(2)	10.7(5)
C2D	9965(3)	6415(3)	5246(2)	8.4(5)
C2B	4786(3)	5535(3)	3936(2)	7.7(5)
O72C	4756(3)	7044(3)	1146(3)	39.8(9)
C4A	3528(3)	9901(3)	3887(3)	15.2(6)
C8A	1784(3)	10125(3)	1394(3)	12.4(5)
C5B	4464(3)	3206(3)	2919(2)	10.2(5)
C2A	2830(3)	8096(3)	2407(2)	10.4(5)

C4B	3607(3)	3571(3)	3318(2)	10.5(5)
C8B	6439(3)	3783(3)	2655(2)	8.1(5)
C3A	3445(3)	8723(3)	3472(2)	13.3(6)
C3B	3768(3)	4752(3)	3834(2)	10.1(5)
C7A	2623(3)	6826(3)	1834(2)	13.7(6)
C3D	11142(3)	6413(3)	5649(2)	10.0(5)
C5A	2988(3)	10394(3)	3239(3)	14.3(6)
C6C	7961(3)	9556(3)	4198(3)	13.5(6)
C7D	9071(3)	6320(3)	5784(2)	10.1(5)
C2C	6416(3)	8451(3)	2627(3)	19.4(7)
C8C	8795(3)	9524(3)	5162(2)	11.2(5)
C7C	5647(4)	7227(3)	1902(3)	21.1(7)
C5D	11414(3)	6575(3)	4121(2)	10.4(5)
C4C	7073(5)	10503(4)	3171(4)	46.4(16)
C3C	6302(5)	9421(4)	2435(4)	41.4(14)
C5C	7918(4)	10572(3)	4063(3)	28.7(9)
O1S	-1257(3)	9217(2)	771(2)	21.5(5)
O5S	4883(3)	4155(3)	628(3)	33.6(7)
O3S	9839(3)	11028(3)	2731(3)	38.0(8)
O2S	5490(4)	9411(3)	-1028(3)	40.1(8)
O4S	6330(5)	8211(5)	36(4)	60.5(12)
O6S	2551(3)	4150(3)	1268(3)	31.7(7)
O7S	2675(3)	4121(3)	-534(3)	33.5(7)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Tb-IV. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	4.94(5)	6.21(5)	6.65(5)	2.61(4)	0.99(4)	1.39(3)
Tb1	7.98(6)	7.74(6)	4.80(6)	2.45(5)	1.10(5)	2.49(5)
O72B	11.1(10)	13.6(10)	14.2(11)	3.6(9)	6.2(8)	6.0(8)
O81A	15.1(11)	10.8(10)	9.8(10)	4.8(8)	2.5(8)	3.8(8)
O1W	13(1)	18.8(11)	10.5(10)	8.6(9)	5.0(8)	6.6(9)
O82A	32.6(15)	9.6(11)	15.3(12)	2.5(9)	-2.9(11)	8.2(10)
O3W	13.2(10)	18.5(11)	10.8(10)	8.4(9)	3.4(8)	7.9(9)
O71A	30.9(14)	13.4(11)	7.5(10)	2.0(9)	0.2(10)	13(1)
O82B	10.9(10)	9(1)	14.9(10)	3.8(8)	5.1(8)	4.3(8)
O81B	8.9(9)	8.2(9)	11.9(10)	3.5(8)	4.6(8)	1.9(8)
O81D	8.7(9)	12.1(10)	9.8(10)	5.9(8)	2.2(8)	2.5(8)
O72D	17.6(12)	37.3(15)	9.5(11)	11.8(11)	6.2(9)	12.8(11)
O71B	8.9(10)	8.0(9)	14.7(10)	1.6(8)	5.0(8)	1.5(8)
O71D	8.4(9)	15.3(10)	10(1)	7.6(8)	3.3(8)	4.2(8)
O4W	19.5(12)	13.7(11)	23.0(13)	4.7(10)	9.1(10)	0.0(9)
O82D	12.7(10)	13.7(10)	10.4(10)	6.4(8)	5.3(8)	3.1(8)
N1C	11.1(11)	7.4(11)	9.1(11)	2.1(9)	-0.2(9)	2.2(9)
O82C	16.5(11)	12.4(11)	11.4(11)	0.0(9)	-1.2(9)	-1.2(9)
O72A	32.2(14)	15.7(11)	8.7(10)	4.4(9)	1.8(10)	15.5(11)

N1A	10.2(11)	8.8(11)	8.1(11)	3.2(9)	1.7(9)	3.9(9)
O5W	28.2(14)	12.2(11)	26.6(14)	3.8(10)	19.6(12)	5.2(10)
O81C	11.6(10)	11.3(10)	10.7(10)	4.8(8)	1.0(8)	1.9(8)
O3AA	10.6(10)	8.7(10)	11.8(10)	2.2(8)	-1.1(8)	3.8(8)
O6W	13.1(11)	43.1(16)	13.6(11)	17.6(11)	7.4(9)	15.8(11)
O2W	10.6(10)	11.6(10)	15.5(11)	4.9(9)	2.4(8)	3.6(8)
N1D	7.1(10)	7.7(10)	7.3(10)	3.2(9)	2.3(8)	1.9(8)
N1B	7.2(10)	7.9(11)	7.1(10)	3.1(9)	2.0(8)	2.8(8)
C6D	8.2(12)	8.5(12)	7.0(12)	3(1)	2.7(10)	2.0(9)
C6A	12.5(13)	8.2(12)	9.0(13)	2.6(10)	0.9(10)	2.4(10)
C7B	8.1(12)	10.3(12)	7.3(12)	2.7(10)	0.7(10)	2.5(10)
C6B	7.3(12)	8.7(12)	7.6(12)	3.9(10)	2.1(9)	3.1(10)
C8D	9.9(12)	6.8(12)	8.7(12)	3.1(10)	1.7(10)	0.3(10)
C4D	8.0(12)	11.3(13)	11.5(13)	3.7(11)	2(1)	4.3(10)
C2D	8.9(12)	9.1(12)	7.2(12)	3.2(10)	2.5(10)	2.9(10)
C2B	6.2(11)	8.6(12)	6.3(11)	2.0(9)	0.5(9)	2.4(9)
O72C	46(2)	16.5(13)	29.3(16)	3.4(12)	-20.8(15)	9.7(13)
C4A	18.0(15)	13.5(14)	7.9(13)	1.4(11)	-0.1(11)	3.0(12)
C8A	12.7(13)	10.0(13)	12.1(13)	4.8(11)	1.0(11)	2.4(11)
C5B	9.6(12)	9.1(12)	11.7(13)	4.3(10)	4.1(10)	1.6(10)
C2A	12.4(13)	10.8(13)	7.7(12)	3.9(10)	2(1)	5.1(10)
C4B	8.3(12)	12.0(13)	10.4(13)	4.3(11)	3.8(10)	0.7(10)
C8B	7.5(12)	9.1(12)	7.5(12)	3.7(10)	1.7(10)	3.1(10)
C3A	15.2(14)	13.7(14)	8.2(13)	3.9(11)	0.2(11)	4.9(11)
C3B	8.3(12)	12.0(13)	11.2(13)	5.6(11)	4.4(10)	2.7(10)
C7A	20.4(15)	11.4(13)	8.5(13)	2.7(11)	2.3(11)	9.7(12)
C3D	9.2(12)	11.2(13)	8.0(12)	2.9(10)	1.2(10)	4(1)
C5A	17.9(15)	8.9(13)	9.9(13)	1.3(11)	0.0(11)	2.2(11)
C6C	14.4(14)	8.3(13)	12.3(14)	2.4(11)	0.0(11)	1.4(11)
C7D	9.4(12)	12.8(13)	8.1(12)	3.9(10)	3(1)	3.6(10)
C2C	23.8(17)	7.4(13)	15.5(15)	2.3(12)	-7.0(13)	3.8(12)
C8C	10.4(13)	9.9(13)	10.1(13)	2.5(11)	2(1)	1.3(10)
C7C	24.8(18)	8.7(14)	16.8(16)	1.8(12)	-7.8(13)	5.2(13)
C5D	8.7(12)	11.5(13)	11.9(13)	4.6(11)	5(1)	3.5(10)
C4C	63(4)	10.1(17)	34(2)	8.0(17)	-23(2)	1.5(19)
C3C	56(3)	11.8(17)	27(2)	4.3(15)	-23(2)	5.6(18)
C5C	37(2)	7.6(14)	23.4(19)	3.6(13)	-10.1(16)	0.7(14)

Table 4 Bond Lengths for U-Tb-IV.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O81B	2.452(2)		N1A	C6A	1.336(4)
U1	O81D	2.408(2)		N1A	C2A	1.336(4)
U1	O71B	2.312(2)		O81C	C8C	1.295(4)
U1	O71D	2.359(2)		O3AA	C7C	1.277(4)
U1	N1C	2.530(3)		N1D	C6D	1.339(4)
U1	O81C	2.340(2)		N1D	C2D	1.333(4)

U1	O3AA	2.428(2)		N1B	C6B	1.342(4)
U1	N1D	2.542(3)		N1B	C2B	1.337(4)
U1	N1B	2.552(3)		C6D	C8D	1.513(4)
Tb1	O81A	2.386(2)		C6D	C5D	1.389(4)
Tb1	O1W	2.409(2)		C6A	C8A	1.511(4)
Tb1	O3W	2.452(2)		C6A	C5A	1.393(4)
Tb1	O71A	2.469(2)		C7B	C2B	1.507(4)
Tb1	O4W	2.448(3)		C6B	C5B	1.390(4)
Tb1	N1A	2.525(3)		C6B	C8B	1.505(4)
Tb1	O5W	2.402(3)		C4D	C3D	1.395(4)
Tb1	O6W	2.414(3)		C4D	C5D	1.392(4)
Tb1	O2W	2.426(2)		C2D	C3D	1.390(4)
O72B	C7B	1.225(4)		C2D	C7D	1.512(4)
O81A	C8A	1.272(4)		C2B	C3B	1.388(4)
O82A	C8A	1.245(4)		O72C	C7C	1.237(4)
O71A	C7A	1.237(4)		C4A	C3A	1.395(5)
O82B	C8B	1.238(4)		C4A	C5A	1.389(5)
O81B	C8B	1.290(4)		C5B	C4B	1.395(4)
O81D	C8D	1.274(4)		C2A	C3A	1.390(4)
O72D	C7D	1.233(4)		C2A	C7A	1.492(4)
O71B	C7B	1.300(4)		C4B	C3B	1.391(4)
O71D	C7D	1.281(4)		C6C	C8C	1.511(5)
O82D	C8D	1.243(4)		C6C	C5C	1.387(5)
N1C	C6C	1.332(4)		C2C	C7C	1.510(5)
N1C	C2C	1.337(4)		C2C	C3C	1.383(5)
O82C	C8C	1.228(4)		C4C	C3C	1.396(6)
O72A	C7A	1.299(4)		C4C	C5C	1.385(6)

II.23 U-Tb-V

Table 1 Crystal data and structure refinement for U-Tb-V.	
Identification code	U-Tb-V
Empirical formula	$C_{84}H_{56}N_{12}O_{80}Tb_2U_4$
Formula weight	3783.36
Temperature/K	100.0
Crystal system	triclinic
Space group	P-1
a/Å	14.3055(8)
b/Å	16.0001(10)
c/Å	17.1078(10)
α/°	114.756(3)
β/°	113.906(3)
γ/°	92.050(3)
Volume/Å^3	3149.7(3)
Z	1

ρ_{calc}g/cm^3	1.995
μ/mm^{-1}	6.345
F(000)	1782.0
Crystal size/mm^3	0.225 × 0.178 × 0.134
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.892 to 56.806
Index ranges	-19 ≤ h ≤ 19, -21 ≤ k ≤ 21, -22 ≤ l ≤ 22
Reflections collected	94183
Independent reflections	14813 [R_{int} = 0.0673, R_{sigma} = 0.0620]
Data/restraints/parameters	14813/0/770
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0579, wR_2 = 0.1350
Final R indexes [all data]	R_1 = 0.0827, wR_2 = 0.1466
Largest diff. peak/hole / e Å^{-3}	5.16/-4.18

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Tb-V. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	4929.4(3)	6302.7(3)	3131.5(2)	15.45(9)
U2	8449.8(3)	2289.5(3)	1275.0(2)	17.5(1)
Tb3	6316.2(4)	2527.1(4)	3653.0(3)	18.15(11)
O1W	7774(5)	3749(5)	4148(5)	21.8(16)
O2W	7848(7)	1998(7)	4235(7)	38(2)
O3W	6040(8)	942(6)	2398(7)	42(2)
O4W	5861(7)	1498(7)	4191(6)	37(2)
O5W	4458(6)	1983(5)	2806(5)	24.6(16)
O71A	3879(5)	7331(5)	2797(5)	21.2(15)
O71B	4094(5)	5207(5)	1503(4)	18.7(15)
O71C	4956(5)	4786(5)	3168(5)	19.6(15)
O71D	10206(5)	2440(5)	1559(5)	21.8(15)
O71E	9231(5)	3904(5)	2578(5)	22.8(16)
O71F	7247(6)	2265(5)	1907(5)	23.2(16)
O72A	3340(6)	8304(6)	2153(6)	31.9(19)
O72B	2795(6)	4048(6)	106(5)	29.6(18)
O72C	5609(5)	3902(5)	3877(5)	19.5(15)
O72D	11487(6)	2131(6)	1132(6)	35(2)
O72E	10430(6)	4979(6)	4068(5)	30.1(18)
O72F	5950(5)	2712(5)	2264(5)	19.2(15)
O81A	6444(5)	6036(5)	2890(5)	21.6(15)
O81B	4218(5)	6651(5)	4239(5)	22.0(16)
O81C	6080(5)	7825(5)	4409(5)	19.3(15)
O81D	6933(5)	1158(5)	-156(5)	23.8(16)
O81E	8501(6)	898(6)	1419(6)	31.4(18)
O81F	8471(5)	3096(5)	394(5)	21.3(15)
O82A	7623(6)	6286(7)	2418(7)	38(2)
O82B	2903(5)	6570(5)	4623(5)	21.0(15)

O82C	7339(7)	8810(6)	5917(6)	36(2)
O82D	6108(6)	-91(6)	-1642(6)	31.1(19)
O82E	8855(9)	60(8)	2225(8)	56(3)
O82F	7791(6)	3877(6)	-443(5)	29.7(18)
N1A	5409(6)	7167(6)	2350(5)	18.2(17)
N1B	3031(6)	5429(6)	2430(6)	18.4(18)
N1C	6291(6)	6357(6)	4685(5)	16.2(17)
N1D	8769(6)	1142(6)	-96(6)	18.8(17)
N1E	9506(7)	2501(7)	2973(6)	23.3(19)
N1F	7006(6)	3147(6)	908(5)	16.7(17)
C2A	4836(8)	7739(8)	2106(8)	24(2)
C2B	2518(7)	4780(7)	1507(7)	15.9(19)
C2C	6355(7)	5554(7)	4761(6)	15.3(19)
C2D	9743(7)	1194(8)	-8(7)	20(2)
C2E	10020(8)	3371(9)	3734(8)	27(2)
C2F	6281(7)	3144(7)	1217(6)	17(2)
C3A	5092(9)	8234(9)	1702(8)	32(3)
C3B	1479(8)	4264(9)	1095(7)	26(2)
C3C	7067(8)	5561(8)	5610(7)	23(2)
C3D	9959(8)	610(8)	-741(8)	28(2)
C3E	10601(9)	3494(10)	4664(8)	36(3)
C3F	5478(8)	3600(8)	1025(7)	20(2)
C4A	5942(10)	8116(10)	1524(10)	39(3)
C4B	990(8)	4480(9)	1675(8)	30(3)
C4C	7688(8)	6438(8)	6417(7)	24(2)
C4D	9112(9)	-69(9)	-1614(9)	34(3)
C4E	10652(10)	2706(11)	4809(9)	41(3)
C4F	5415(8)	4055(8)	485(7)	23(2)
C5A	6536(9)	7529(9)	1768(8)	29(2)
C5B	1525(9)	5149(9)	2644(9)	29(3)
C5C	7611(8)	7247(8)	6338(7)	24(2)
C5D	8088(9)	-132(8)	-1711(7)	28(2)
C5E	10121(10)	1826(10)	4033(9)	36(3)
C5F	6175(8)	4081(8)	173(7)	24(2)
C6A	6243(8)	7060(8)	2183(7)	23(2)
C6B	2565(7)	5617(8)	2998(7)	18(2)
C6C	6910(7)	7189(7)	5451(6)	18(2)
C6D	7946(8)	488(8)	-942(7)	23(2)
C6E	9548(10)	1741(10)	3117(9)	35(3)
C6F	6944(7)	3603(7)	392(6)	17(2)
C7A	3935(7)	7803(8)	2357(7)	20(2)
C7B	3150(8)	4636(8)	959(7)	19(2)
C7C	5590(7)	4662(8)	3867(7)	18(2)
C7D	10580(8)	1972(8)	969(8)	22(2)
C7E	9910(8)	4166(8)	3468(7)	23(2)
C7F	6482(7)	2666(7)	1845(7)	17(2)
C8A	6835(8)	6408(8)	2508(7)	24(2)
C8B	3273(7)	6341(8)	4035(7)	20(2)

C8C	6787(8)	8016(8)	5267(7)	22(2)
C8D	6912(8)	508(8)	-928(7)	25(2)
C8E	8918(10)	811(9)	2196(10)	35(3)
C8F	7802(7)	3538(8)	84(7)	20(2)
O1S	7682(6)	4794(5)	3238(5)	24.1(15)
O2S	3539(6)	2922(6)	1812(5)	27.3(16)
O3S	7211(7)	1900(7)	6089(7)	42(2)
O4S	4227(8)	121(8)	3716(7)	51(2)
O5S	8799(9)	3309(8)	-1490(8)	62(3)
O6S	-702(9)	5610(9)	2461(8)	64(3)
O7S	599(9)	4359(9)	-945(8)	63(3)
O8S	9127(10)	2692(9)	6213(9)	72(3)
O9S	8610(11)	7763(10)	1194(10)	85(4)
O10S	8324(10)	10565(9)	6345(9)	74(3)
O11S	6029(11)	91(10)	577(10)	87(4)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Tb-V. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	13.37(16)	23.9(2)	9.81(15)	9.18(15)	4.98(13)	2.39(13)
U2	15.74(17)	23.7(2)	11.96(16)	7.13(15)	7.02(13)	2.29(13)
Tb3	21.4(2)	22.8(3)	15.7(2)	11.0(2)	11.69(18)	2.82(18)
O1W	17(3)	31(5)	16(3)	12(3)	6(3)	-1(3)
O2W	47(5)	36(6)	53(5)	31(5)	31(4)	19(4)
O3W	71(7)	32(6)	47(5)	21(4)	45(5)	18(4)
O4W	49(5)	41(6)	44(5)	30(4)	30(4)	13(4)
O5W	30(4)	18(4)	22(4)	7(3)	13(3)	-2(3)
O71A	19(3)	28(5)	19(3)	14(3)	8(3)	8(3)
O71B	15(3)	30(4)	11(3)	10(3)	6(3)	0(3)
O71C	16(3)	25(4)	12(3)	8(3)	3(3)	4(3)
O71D	19(3)	25(4)	13(3)	5(3)	4(3)	-1(3)
O71E	22(4)	27(5)	15(3)	8(3)	7(3)	2(3)
O71F	30(4)	28(5)	22(4)	15(3)	19(3)	9(3)
O72A	22(4)	39(5)	36(4)	22(4)	10(3)	10(3)
O72B	30(4)	35(5)	15(3)	5(3)	10(3)	-3(3)
O72C	17(3)	27(5)	16(3)	12(3)	8(3)	4(3)
O72D	16(4)	40(6)	31(4)	3(4)	10(3)	4(3)
O72E	23(4)	37(5)	13(3)	3(3)	3(3)	-2(3)
O72F	20(3)	27(4)	14(3)	12(3)	10(3)	3(3)
O81A	21(3)	31(5)	24(4)	18(3)	15(3)	7(3)
O81B	20(3)	30(5)	16(3)	11(3)	7(3)	2(3)
O81C	20(3)	20(4)	16(3)	12(3)	4(3)	3(3)
O81D	17(3)	22(4)	28(4)	7(3)	12(3)	2(3)
O81E	32(4)	32(5)	32(4)	14(4)	18(4)	9(3)
O81F	13(3)	35(5)	19(3)	13(3)	10(3)	4(3)
O82A	33(4)	55(6)	56(6)	39(5)	34(4)	25(4)

O82B	26(4)	30(4)	16(3)	13(3)	15(3)	6(3)
O82C	40(5)	22(5)	27(4)	11(4)	0(4)	0(4)
O82D	19(4)	17(5)	34(4)	-2(3)	8(3)	-3(3)
O82E	75(7)	52(7)	80(8)	45(6)	53(7)	31(6)
O82F	30(4)	50(6)	29(4)	29(4)	20(3)	12(4)
N1A	15(4)	25(5)	12(4)	7(3)	6(3)	2(3)
N1B	11(4)	34(5)	15(4)	15(4)	7(3)	4(3)
N1C	15(4)	21(5)	12(4)	8(3)	6(3)	0(3)
N1D	19(4)	22(5)	14(4)	7(3)	7(3)	1(3)
N1E	26(4)	33(6)	22(4)	17(4)	16(4)	12(4)
N1F	15(4)	23(5)	13(4)	8(3)	8(3)	-1(3)
C2A	22(5)	24(6)	24(5)	11(5)	9(4)	4(4)
C2B	21(5)	24(6)	16(4)	17(4)	12(4)	12(4)
C2C	13(4)	16(5)	13(4)	6(4)	4(3)	4(3)
C2D	15(4)	27(6)	19(5)	13(4)	8(4)	6(4)
C2E	15(5)	44(8)	22(5)	17(5)	7(4)	5(4)
C2F	17(4)	23(6)	9(4)	6(4)	7(3)	-1(4)
C3A	27(6)	45(8)	35(6)	30(6)	11(5)	11(5)
C3B	19(5)	41(7)	17(5)	17(5)	4(4)	3(4)
C3C	19(5)	23(6)	17(5)	9(4)	2(4)	-1(4)
C3D	19(5)	30(7)	31(6)	8(5)	16(4)	3(4)
C3E	29(6)	53(9)	24(6)	18(6)	12(5)	8(5)
C3F	20(5)	35(7)	17(4)	17(5)	13(4)	10(4)
C4A	44(7)	51(9)	51(8)	38(7)	33(6)	17(6)
C4B	24(5)	47(8)	22(5)	22(5)	9(4)	-2(5)
C4C	20(5)	26(6)	14(4)	8(4)	-1(4)	0(4)
C4D	25(6)	41(8)	29(6)	8(5)	15(5)	8(5)
C4E	38(7)	72(11)	27(6)	35(7)	15(5)	21(7)
C4F	27(5)	36(7)	18(5)	20(5)	14(4)	17(5)
C5A	30(6)	34(7)	37(6)	22(6)	24(5)	10(5)
C5B	32(6)	38(7)	45(7)	34(6)	28(5)	18(5)
C5C	23(5)	27(7)	16(5)	7(4)	7(4)	3(4)
C5D	26(5)	28(7)	17(5)	4(5)	7(4)	3(4)
C5E	40(7)	49(9)	37(7)	31(7)	22(6)	20(6)
C5F	27(5)	34(7)	14(4)	11(4)	13(4)	7(4)
C6A	26(5)	28(7)	20(5)	15(5)	11(4)	6(4)
C6B	21(5)	29(6)	12(4)	14(4)	10(4)	12(4)
C6C	12(4)	22(6)	12(4)	3(4)	3(3)	2(4)
C6D	20(5)	26(6)	17(5)	8(4)	6(4)	2(4)
C6E	40(7)	51(9)	40(7)	29(6)	32(6)	26(6)
C6F	13(4)	26(6)	8(4)	6(4)	4(3)	-3(4)
C7A	12(4)	20(6)	17(4)	6(4)	1(4)	4(4)
C7B	21(5)	30(6)	17(4)	16(4)	12(4)	6(4)
C7C	14(4)	23(6)	18(4)	11(4)	8(4)	2(4)
C7D	17(5)	21(6)	27(5)	12(5)	8(4)	6(4)
C7E	18(5)	29(7)	19(5)	9(5)	9(4)	5(4)
C7F	19(5)	18(6)	13(4)	6(4)	8(4)	1(4)
C8A	24(5)	28(7)	21(5)	12(5)	10(4)	3(4)

C8B	17(4)	30(6)	19(5)	16(4)	9(4)	6(4)
C8C	24(5)	20(6)	14(4)	5(4)	5(4)	1(4)
C8D	22(5)	27(7)	22(5)	8(5)	12(4)	7(4)
C8E	43(7)	32(8)	51(8)	26(6)	33(6)	15(5)
C8F	19(5)	23(6)	13(4)	4(4)	10(4)	-3(4)

Table 4 Bond Lengths for U-Tb-V.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O71A	2.358(7)		O82F	C8F	1.226(12)
U1	O71B	2.307(6)		N1A	C2A	1.334(14)
U1	O71C	2.454(7)		N1A	C6A	1.336(13)
U1	O81A	2.386(7)		N1B	C2B	1.320(12)
U1	O81B	2.378(7)		N1B	C6B	1.331(11)
U1	O81C	2.399(7)		N1C	C2C	1.346(13)
U1	N1A	2.529(8)		N1C	C6C	1.337(12)
U1	N1B	2.540(8)		N1D	C2D	1.335(12)
U1	N1C	2.543(8)		N1D	C6D	1.356(12)
U2	O71D	2.339(7)		N1E	C2E	1.344(15)
U2	O71E	2.417(7)		N1E	C6E	1.338(16)
U2	O71F	2.380(7)		N1F	C2F	1.343(11)
U2	O81D	2.384(7)		N1F	C6F	1.343(12)
U2	O81E	2.341(8)		C2A	C3A	1.372(15)
U2	O81F	2.365(7)		C2A	C7A	1.509(14)
U2	N1D	2.530(8)		C2B	C3B	1.402(14)
U2	N1E	2.533(8)		C2B	C7B	1.506(12)
U2	N1F	2.532(8)		C2C	C3C	1.391(13)
Tb3	O1W	2.403(7)		C2C	C7C	1.510(13)
Tb3	O2W	2.363(8)		C2D	C3D	1.377(14)
Tb3	O3W	2.425(9)		C2D	C7D	1.519(14)
Tb3	O4W	2.379(8)		C2E	C3E	1.383(15)
Tb3	O5W	2.363(7)		C2E	C7E	1.514(16)
Tb3	O72C	2.403(7)		C2F	C3F	1.383(14)
Tb3	O72F	2.366(6)		C2F	C7F	1.507(13)
Tb3	O82B[1]	2.383(7)		C3A	C4A	1.370(16)
O71A	C7A	1.289(12)		C3B	C4B	1.373(15)
O71B	C7B	1.306(12)		C3C	C4C	1.400(14)
O71C	C7C	1.275(11)		C3D	C4D	1.399(16)
O71D	C7D	1.304(12)		C3E	C4E	1.382(19)
O71E	C7E	1.294(12)		C3F	C4F	1.376(13)
O71F	C7F	1.279(12)		C4A	C5A	1.370(17)
O72A	C7A	1.238(12)		C4B	C5B	1.380(16)
O72B	C7B	1.220(12)		C4C	C5C	1.361(16)
O72C	C7C	1.224(12)		C4D	C5D	1.400(15)
O72D	C7D	1.204(12)		C4E	C5E	1.36(2)
O72E	C7E	1.222(13)		C4F	C5F	1.398(14)
O72F	C7F	1.226(11)		C5A	C6A	1.382(14)

O81A	C8A	1.301(12)		C5B	C6B	1.397(14)
O81B	C8B	1.273(11)		C5C	C6C	1.399(13)
O81C	C8C	1.292(11)		C5D	C6D	1.376(15)
O81D	C8D	1.282(13)		C5E	C6E	1.385(16)
O81E	C8E	1.288(15)		C5F	C6F	1.378(15)
O81F	C8F	1.285(13)		C6A	C8A	1.510(15)
O82A	C8A	1.209(13)		C6B	C8B	1.501(14)
O82B	Tb3[1]	2.383(7)		C6C	C8C	1.485(15)
O82B	C8B	1.251(11)		C6D	C8D	1.491(14)
O82C	C8C	1.228(13)		C6E	C8E	1.516(19)
O82D	C8D	1.238(13)		C6F	C8F	1.511(12)
O82E	C8E	1.225(15)				

[1]1-X,1-Y,1-Z

II.24 U-Dy-V

Table 1 Crystal data and structure refinement for U-Dy-V.	
Identification code	U-Dy-V
Empirical formula	$C_{84}H_{56}Dy_2N_{12}O_{78}U_4$
Formula weight	3758.52
Temperature/K	100.01
Crystal system	triclinic
Space group	P-1
a/Å	14.3980(12)
b/Å	16.1097(13)
c/Å	17.0781(15)
α/°	115.169(4)
β/°	113.423(4)
γ/°	92.529(4)
Volume/Å^3	3179.5(5)
Z	1
ρ_{calc}g/cm^3	1.963
μ/mm^{-1}	6.346
F(000)	1768.0
Crystal size/mm^3	0.179 × 0.167 × 0.145
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.89 to 56.706
Index ranges	-19 ≤ h ≤ 19, -21 ≤ k ≤ 21, -22 ≤ l ≤ 22
Reflections collected	82270
Independent reflections	15709 [R_{int} = 0.0315, R_{sigma} = 0.0260]
Data/restraints/parameters	15709/0/766
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0219, wR_2 = 0.0520
Final R indexes [all data]	R_1 = 0.0263, wR_2 = 0.0534

Largest diff. peak/hole / e Å^{-3}	1.81/-0.93

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Dy-V. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	5069.9(2)	8705.6(2)	1874.6(2)	7.43(3)
Dy1	3711.7(2)	12470.0(2)	1371.0(2)	8.47(3)
U2	1562.8(2)	12695.7(2)	3741.8(2)	9.49(3)
N1A	4616(2)	7850.2(18)	2658.1(18)	10.3(5)
C2A	3786(3)	7948(2)	2834(2)	14.2(6)
C3A	3500(3)	7476(3)	3245(3)	22.8(8)
C4A	4088(3)	6877(3)	3476(3)	24.3(8)
C5A	4938(3)	6767(2)	3291(3)	17.6(7)
C6A	5185(2)	7278(2)	2887(2)	11.9(6)
C7A	3192(3)	8589(2)	2513(2)	14.9(6)
C8A	6075(2)	7204(2)	2623(2)	11.4(6)
O71A	3575.4(17)	8971.0(16)	2144.0(16)	13.7(4)
O72A	2394(2)	8698(2)	2608(2)	29.4(6)
O81A	6118.9(17)	7681.7(15)	2184.0(16)	12.5(4)
O82A	6667.4(18)	6713.3(16)	2809.9(17)	16.8(5)
N1B	6953.4(19)	9582.5(17)	2564.3(18)	8.9(5)
C2B	7413(2)	9392(2)	1987(2)	9.9(6)
C3B	8444(2)	9854(2)	2334(2)	12.4(6)
C4B	8998(2)	10545(2)	3311(2)	14.1(6)
C5B	8512(2)	10746(2)	3902(2)	13.5(6)
C6B	7483(2)	10241(2)	3501(2)	10.4(6)
C7B	6697(2)	8672(2)	946(2)	9.7(6)
C8B	6850(2)	10370(2)	4048(2)	12.0(6)
O71B	5761.7(17)	8366.6(15)	751.0(15)	11.9(4)
O72B	7048.8(17)	8448.4(15)	346.1(15)	11.2(4)
O81B	5912.7(16)	9804.2(15)	3516.6(15)	11.4(4)
O82B	7212(2)	10958.1(18)	4908.0(17)	21.9(5)
N1C	3695.2(19)	8651.2(17)	332.0(18)	8.7(5)
C2C	3631(2)	9443(2)	255(2)	9.6(6)
C3C	2929(2)	9429(2)	-591(2)	13.6(6)
C4C	2293(3)	8562(2)	-1394(2)	14.9(6)
C5C	2367(2)	7743(2)	-1319(2)	13.6(6)
C6C	3069(2)	7821(2)	-436(2)	10.5(6)
C7C	4407(2)	10336(2)	1154(2)	8.9(6)
C8C	3196(2)	6987(2)	-258(2)	12.5(6)
O71C	5036.4(16)	10219.5(15)	1851.6(15)	11.1(4)
O72C	4396.4(17)	11103.3(15)	1145.4(16)	11.4(4)
O81C	3913.4(17)	7186.4(15)	593.3(16)	13.0(4)
O82C	2624(2)	6195.3(16)	-908.1(17)	24.3(6)
N1D	1235(2)	13843.5(18)	5112.2(19)	11.3(5)
C2D	2038(2)	14505(2)	5947(2)	13.5(6)
C3D	1894(3)	15132(2)	6719(2)	17.8(7)
C4D	875(3)	15078(2)	6606(3)	20.1(7)

C5D	39(3)	14402(2)	5734(2)	17.0(7)
C6D	259(2)	13787(2)	5002(2)	13.1(6)
C7D	3089(2)	14486(2)	5954(2)	13.7(6)
C8D	-557(2)	13003(2)	4027(2)	13.7(6)
O71D	3071.8(17)	13826.7(16)	5186.6(17)	15.7(5)
O72D	3888.3(18)	15084.7(16)	6678.5(18)	20.3(5)
O81D	-185.3(17)	12535.6(16)	3446.9(16)	14.8(5)
O82D	-1485.2(18)	12856.1(18)	3843.3(19)	23.4(5)
N1E	525(2)	12485.0(19)	2039(2)	13.4(5)
C2E	490(3)	13251(2)	1913(2)	16.4(7)
C3E	-74(3)	13178(3)	999(3)	22.8(8)
C4E	-608(3)	12283(3)	207(3)	23.0(8)
C5E	-571(3)	11492(3)	341(2)	19.5(7)
C6E	7(2)	11625(2)	1274(2)	13.4(6)
C7E	1105(3)	14171(2)	2844(3)	19.3(7)
C8E	97(2)	10825(2)	1520(2)	13.2(6)
O71E	1522.8(19)	14087.8(16)	3618.0(17)	17.5(5)
O72E	1166(2)	14932.0(18)	2834(2)	29.7(6)
O81E	780.6(17)	11073.4(15)	2408.7(16)	13.5(4)
O82E	-447.6(19)	10017.4(17)	906.6(17)	19.0(5)
N1F	3007(2)	11842.0(18)	4098.3(18)	10.8(5)
C2F	3727(2)	11852(2)	3793(2)	11.0(6)
C3F	4533(3)	11410(2)	3987(2)	14.8(6)
C4F	4574(3)	10934(2)	4505(2)	17.5(7)
C5F	3831(3)	10920(2)	4825(2)	15.5(6)
C6F	3056(2)	11391(2)	4611(2)	10.2(6)
C7F	3517(2)	12331(2)	3174(2)	12.0(6)
C8F	2215(2)	11464(2)	4930(2)	12.3(6)
O71F	2765.7(18)	12726.4(16)	3108.8(17)	15.0(5)
O72F	4063.6(17)	12292.4(16)	2753.0(16)	13.4(4)
O81F	1537.0(17)	11877.3(16)	4611.4(16)	13.2(4)
O82F	2236.7(19)	11130.3(17)	5466.0(17)	17.8(5)
O1W	2253.6(17)	11258.9(16)	872.5(16)	13.4(4)
O2W	3981(2)	14044.2(18)	2615(2)	27.6(6)
O3W	2198.3(19)	12991.9(18)	781(2)	22.3(5)
O4W	4189.5(19)	13474.7(16)	833.2(17)	17.2(5)
O5W	5554.9(17)	13001.2(16)	2204.6(16)	15.8(5)
O1S	2342.7(18)	10194.4(16)	1760.5(16)	15.6(5)
O2S	6472.2(19)	12089.0(17)	3213.8(18)	20.0(5)
O3S	2817.9(19)	13095.3(17)	-1055.3(18)	19.6(5)
O4S	702(2)	9371.9(18)	2537.9(19)	24.7(6)
O5S	5779(2)	14874.6(18)	1276.9(19)	23.6(5)
O6S	9425(2)	10611(2)	5911(2)	29.0(6)
O7S	1228(2)	11698(2)	6532(2)	31.4(6)
O8S	917(2)	12305(2)	-1189(2)	29.5(6)
O9S	1371(3)	7243(2)	3803(2)	43.6(8)
O10S	3914(3)	15422(2)	566(2)	42.6(8)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U-Dy-V. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka*b*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	8.00(5)	7.64(5)	7.00(5)	3.83(4)	3.35(4)	2.76(4)
Dy1	11.14(7)	7.81(6)	8.94(7)	4.76(5)	5.99(5)	3.16(5)
U2	9.27(5)	10.44(5)	8.53(5)	3.70(4)	4.83(4)	2.83(4)
N1A	10.5(12)	10.9(12)	8.5(12)	5(1)	3.2(10)	2.8(10)
C2A	17.3(16)	18.1(16)	13.8(15)	9.5(13)	10.9(13)	8.2(13)
C3A	25.7(19)	29(2)	29(2)	18.9(17)	20.5(17)	12.0(15)
C4A	32(2)	29(2)	29(2)	22.7(17)	20.7(17)	10.7(16)
C5A	20.8(17)	17.4(16)	21.2(17)	14.5(14)	9.5(14)	8.3(13)
C6A	13.0(15)	11.1(14)	10.1(14)	5.1(12)	4.0(12)	3.8(11)
C7A	16.7(16)	16.8(16)	15.4(16)	8.7(13)	9.7(13)	8.3(13)
C8A	11.4(14)	10.8(14)	8.7(14)	3.8(12)	2.7(12)	1.9(11)
O71A	14.8(11)	14.8(11)	17.1(12)	10.4(9)	9.3(9)	7.0(9)
O72A	29.9(15)	43.7(17)	48.3(18)	35.1(15)	32.5(14)	26.4(13)
O81A	12.6(11)	14.5(11)	13.2(11)	8.1(9)	6.7(9)	6.6(9)
O82A	14.9(11)	14.9(11)	21.0(12)	10.8(10)	5.8(10)	7.7(9)
N1B	9.7(12)	9.2(12)	8.8(12)	5.3(10)	3.8(10)	3.9(9)
C2B	11.4(14)	9.7(14)	11.6(14)	7.1(12)	5.8(12)	4.7(11)
C3B	14.2(15)	11.7(15)	16.1(16)	8.4(13)	9.1(13)	5.8(12)
C4B	11.6(15)	13.9(15)	16.9(16)	8.8(13)	5.3(13)	2.1(12)
C5B	12.2(15)	14.8(15)	10.7(15)	6.8(12)	2.3(12)	2.6(12)
C6B	11.9(14)	10.5(14)	8.5(14)	5.5(12)	3.2(12)	3.9(11)
C7B	13.5(14)	9.2(14)	12.0(14)	8.1(12)	7.1(12)	6.9(11)
C8B	12.2(15)	14.3(15)	10.5(15)	7.0(12)	4.9(12)	3.8(12)
O71B	12.1(11)	13.3(11)	10.3(11)	5.1(9)	5.8(9)	3.2(8)
O72B	15.6(11)	12(1)	11.9(11)	7.0(9)	9.9(9)	5.7(9)
O81B	11(1)	14.4(11)	8.7(10)	5.3(9)	4.8(9)	3.1(8)
O82B	24.7(13)	22.0(13)	10.4(12)	1.4(10)	8.2(10)	-3.4(10)
N1C	9.1(12)	7.9(12)	8.3(12)	3.5(10)	3.7(10)	2.4(9)
C2C	10.0(14)	8.5(14)	12.3(15)	5.6(12)	6.3(12)	3.1(11)
C3C	15.3(15)	11.5(15)	11.6(15)	6.5(12)	2.9(13)	2.8(12)
C4C	16.0(16)	15.0(15)	9.8(15)	6.3(13)	2.1(13)	3.6(12)
C5C	13.9(15)	12.3(15)	11.2(15)	4.6(12)	4.0(12)	1.9(12)
C6C	11.4(14)	9.7(14)	9.8(14)	3.8(12)	5.1(12)	3.4(11)
C7C	9.0(14)	8.7(14)	10.6(14)	3.9(11)	6.5(12)	2.8(11)
C8C	16.7(15)	9.9(14)	11.5(15)	6.2(12)	5.9(13)	4.0(12)
O71C	12.0(11)	8.7(10)	10(1)	4.9(8)	2.5(9)	1.6(8)
O72C	12.4(11)	7.1(10)	13.1(11)	4.7(9)	4.6(9)	2.5(8)
O81C	16.5(11)	8.5(10)	11.0(11)	4.9(9)	3.5(9)	1.7(8)
O82C	35.8(15)	8.8(11)	12.7(12)	3.8(9)	-0.4(11)	-2.2(10)
N1D	10.3(12)	11.2(12)	12.6(13)	5.6(10)	5.6(10)	2.6(10)
C2D	13.2(15)	12.6(15)	15.4(16)	6.6(13)	7.1(13)	4.9(12)
C3D	18.4(17)	13.0(16)	15.2(16)	2.0(13)	6.9(14)	1.9(13)
C4D	22.1(18)	19.0(17)	18.4(17)	4.1(14)	13.7(15)	7.0(14)
C5D	16.6(16)	16.9(16)	19.4(17)	6.6(14)	12.2(14)	5.0(13)

C6D	14.8(15)	10.9(14)	15.1(16)	6.6(12)	8.0(13)	2.9(12)
C7D	11.9(15)	10.2(14)	15.7(16)	5.0(12)	4.7(13)	2.1(12)
C8D	12.7(15)	13.1(15)	16.2(16)	6.9(13)	7.5(13)	3.3(12)
O71D	13.0(11)	13.0(11)	17.0(12)	3.4(9)	7.6(10)	3.0(9)
O72D	11.0(11)	12.2(11)	23.5(13)	1.8(10)	3(1)	-1.0(9)
O81D	11.5(11)	15.3(11)	13.9(11)	3.7(9)	6.4(9)	2.3(9)
O82D	11.6(12)	24.2(13)	25.6(14)	4.9(11)	8.7(11)	2(1)
N1E	13.6(13)	15.6(13)	15.3(14)	8.7(11)	9.1(11)	6.2(10)
C2E	18.0(16)	21.6(17)	19.5(17)	13.2(14)	13.4(14)	10.7(13)
C3E	29(2)	31(2)	25.0(19)	22.7(17)	17.2(16)	16.7(16)
C4E	24.9(19)	36(2)	16.6(17)	18.2(16)	10.3(15)	13.2(16)
C5E	16.2(16)	27.9(19)	12.8(16)	9.0(14)	6.0(14)	8.5(14)
C6E	11.7(15)	18.2(16)	13.7(15)	8.3(13)	7.9(13)	7.6(12)
C7E	22.3(18)	19.1(17)	28.6(19)	14.5(15)	18.7(16)	12.3(14)
C8E	12.4(15)	17.0(16)	12.9(15)	6.6(13)	8.7(13)	6.4(12)
O71E	23.3(13)	11.7(11)	18.9(12)	6.4(10)	12(1)	7.0(9)
O72E	46.2(17)	19.6(13)	38.6(16)	18.9(12)	27.5(14)	15.2(12)
O81E	15.3(11)	13.0(11)	9.4(11)	4.4(9)	4.3(9)	4.7(9)
O82E	19.7(12)	16.5(12)	13.9(12)	3.6(10)	5.8(10)	2.4(10)
N1F	11.6(12)	11.4(12)	7.8(12)	3.5(10)	4.3(10)	2.2(10)
C2F	13.3(15)	12.4(14)	8.2(14)	4.1(12)	6.5(12)	3.8(12)
C3F	16.2(16)	17.7(16)	14.0(16)	8.0(13)	9.6(13)	6.3(13)
C4F	21.4(17)	20.2(17)	20.2(17)	12.4(14)	14.3(14)	12.1(14)
C5F	18.7(16)	17.0(16)	15.7(16)	10.7(13)	9.1(14)	6.9(13)
C6F	12.5(15)	9.3(14)	5.8(13)	1.6(11)	4.1(12)	-0.2(11)
C7F	13.6(15)	11.1(14)	8.7(14)	3.5(12)	4.5(12)	1.3(12)
C8F	13.9(15)	10.1(14)	8.4(14)	1.8(12)	4.5(12)	-1.9(11)
O71F	17.2(12)	19.4(12)	17.1(12)	12.2(10)	11.5(10)	9.3(9)
O72F	12.6(11)	18.3(11)	11.0(11)	7.3(9)	6.9(9)	3.3(9)
O81F	11.4(11)	17.9(11)	12.5(11)	8.5(9)	6.5(9)	3.4(9)
O82F	22.0(12)	22.7(12)	17.5(12)	13.3(10)	13(1)	6.4(10)
O1W	12.2(11)	17.2(11)	14.7(11)	10.6(9)	6.6(9)	3.1(9)
O2W	50.8(18)	17.3(13)	31.3(15)	11.9(11)	32.8(14)	16.4(12)
O3W	20.9(13)	24.8(13)	37.0(15)	21.8(12)	19.1(12)	14.2(10)
O4W	22.9(13)	14.3(11)	17.4(12)	10.4(10)	9(1)	3.9(9)
O5W	16.7(12)	9.6(11)	16.2(12)	5.5(9)	4.5(10)	-0.8(9)

Table 4 Bond Lengths for U-Dy-V.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	N1A	2.510(3)		O72B	$Dy1^{1}$	2.367(2)
U1	O71A	2.393(2)		N1C	C2C	1.340(4)
U1	O81A	2.368(2)		N1C	C6C	1.336(4)
U1	N1B	2.539(3)		C2C	C3C	1.384(4)
U1	O71B	2.377(2)		C2C	C7C	1.514(4)
U1	O81B	2.313(2)		C3C	C4C	1.389(4)
U1	N1C	2.551(2)		C4C	C5C	1.384(4)

U1	O71C	2.458(2)		C5C	C6C	1.388(4)
U1	O81C	2.396(2)		C6C	C8C	1.502(4)
Dy1	O72B[1]	2.367(2)		C7C	O71C	1.274(4)
Dy1	O72C	2.396(2)		C7C	O72C	1.243(4)
Dy1	O72F	2.355(2)		C8C	O81C	1.289(4)
Dy1	O1W	2.397(2)		C8C	O82C	1.230(4)
Dy1	O2W	2.402(2)		N1D	C2D	1.339(4)
Dy1	O3W	2.368(2)		N1D	C6D	1.336(4)
Dy1	O4W	2.367(2)		C2D	C3D	1.380(4)
Dy1	O5W	2.358(2)		C2D	C7D	1.511(4)
U2	N1D	2.528(3)		C3D	C4D	1.396(5)
U2	O71D	2.386(2)		C4D	C5D	1.390(5)
U2	O81D	2.341(2)		C5D	C6D	1.390(4)
U2	N1E	2.543(3)		C6D	C8D	1.508(4)
U2	O71E	2.341(2)		C7D	O71D	1.279(4)
U2	O81E	2.434(2)		C7D	O72D	1.241(4)
U2	N1F	2.558(3)		C8D	O81D	1.287(4)
U2	O71F	2.387(2)		C8D	O82D	1.231(4)
U2	O81F	2.377(2)		N1E	C2E	1.339(4)
N1A	C2A	1.344(4)		N1E	C6E	1.333(4)
N1A	C6A	1.339(4)		C2E	C3E	1.391(5)
C2A	C3A	1.378(5)		C2E	C7E	1.507(5)
C2A	C7A	1.510(4)		C3E	C4E	1.384(5)
C3A	C4A	1.390(5)		C4E	C5E	1.387(5)
C4A	C5A	1.381(5)		C5E	C6E	1.384(4)
C5A	C6A	1.390(4)		C6E	C8E	1.513(4)
C6A	C8A	1.512(4)		C7E	O71E	1.285(4)
C7A	O71A	1.288(4)		C7E	O72E	1.233(4)
C7A	O72A	1.232(4)		C8E	O81E	1.302(4)
C8A	O81A	1.296(4)		C8E	O82E	1.226(4)
C8A	O82A	1.230(4)		N1F	C2F	1.336(4)
N1B	C2B	1.335(4)		N1F	C6F	1.339(4)
N1B	C6B	1.334(4)		C2F	C3F	1.390(4)
C2B	C3B	1.393(4)		C2F	C7F	1.505(4)
C2B	C7B	1.501(4)		C3F	C4F	1.383(5)
C3B	C4B	1.394(4)		C4F	C5F	1.384(5)
C4B	C5B	1.385(5)		C5F	C6F	1.392(4)
C5B	C6B	1.393(4)		C6F	C8F	1.503(4)
C6B	C8B	1.508(4)		C7F	O71F	1.270(4)
C7B	O71B	1.270(4)		C7F	O72F	1.247(4)
C7B	O72B	1.245(4)		C8F	O81F	1.279(4)
C8B	O81B	1.300(4)		C8F	O82F	1.235(4)
C8B	O82B	1.220(4)				

[1]1-X,2-Y,-Z

II.25 U-Ho-V

Table 1 Crystal data and structure refinement for U-Ho-V.	
Identification code	U-Ho-V
Empirical formula	$C_{84}H_{56}Ho_2N_{12}O_{76}U_4$
Formula weight	3731.38
Temperature/K	99.96
Crystal system	triclinic
Space group	P-1
a/Å	14.3644(8)
b/Å	16.1152(9)
c/Å	17.0972(9)
α/°	115.0950(10)
β/°	113.7020(10)
γ/°	92.322(2)
Volume/Å^3	3173.8(3)
Z	1
ρ_{calc}g/cm^3	1.952
μ/mm^{-1}	6.425
F(000)	1754.0
Crystal size/mm^3	0.239 × 0.156 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.886 to 60.978
Index ranges	-20 ≤ h ≤ 20, -23 ≤ k ≤ 22, -23 ≤ l ≤ 24
Reflections collected	101434
Independent reflections	19232 [R_{int} = 0.0373, R_{sigma} = 0.0290]
Data/restraints/parameters	19232/0/762
Goodness-of-fit on F^2	1.021
Final R indexes [I>=2σ (I)]	R_1 = 0.0232, wR_2 = 0.0541
Final R indexes [all data]	R_1 = 0.0295, wR_2 = 0.0563
Largest diff. peak/hole / e Å^{-3}	1.87/-1.01

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Ho-V. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	5068.7(2)	8703.4(2)	1872.8(2)	7.58(2)
Ho1	3702.8(2)	12462.3(2)	1363.8(2)	8.71(3)
U2	1558.2(2)	12699.3(2)	3738.2(2)	9.91(2)
N1A	4616.9(18)	7847.7(17)	2659.4(17)	11.0(4)
C2A	3790(2)	7951(2)	2836(2)	14.1(5)
C3A	3505(3)	7478(3)	3253(3)	24.3(7)
C4A	4090(3)	6874(3)	3480(3)	24.3(7)
C5A	4943(3)	6765(2)	3291(2)	18.7(6)
C6A	5186(2)	7273(2)	2885(2)	12.9(5)

C7A	3192(2)	8592(2)	2517(2)	15.3(6)
C8A	6076(2)	7198(2)	2620(2)	12.1(5)
O71A	3570.0(16)	8968.8(15)	2143.9(15)	13.1(4)
O72A	2398(2)	8702(2)	2613(2)	29.6(6)
O81A	6120.8(15)	7678.1(14)	2182.9(14)	11.6(4)
O82A	6668.1(16)	6706.6(15)	2808.5(16)	16.7(4)
N1B	6952.6(17)	9577.0(16)	2560.9(16)	8.9(4)
C2B	7417(2)	9389(2)	1985.4(19)	10.2(5)
C3B	8446(2)	9853(2)	2332(2)	11.7(5)
C4B	9000(2)	10541(2)	3307(2)	13.3(5)
C5B	8512(2)	10742(2)	3898(2)	13.4(5)
C6B	7484(2)	10233(2)	3496(2)	11.2(5)
C7B	6695(2)	8671(2)	945(2)	10.7(5)
C8B	6850(2)	10367(2)	4047(2)	11.9(5)
O71B	5760.5(15)	8366.7(14)	749.9(14)	12.2(4)
O72B	7048.3(16)	8445.3(14)	340.8(14)	11.6(4)
O81B	5913.2(15)	9803.5(15)	3515.1(14)	11.8(4)
O82B	7216.0(18)	10950.6(17)	4907.0(15)	21.9(5)
N1C	3692.5(18)	8651.5(16)	330.6(16)	8.8(4)
C2C	3627(2)	9446.0(19)	254.8(19)	9.8(5)
C3C	2927(2)	9429(2)	-593(2)	14.3(5)
C4C	2290(2)	8563(2)	-1401(2)	15.2(5)
C5C	2368(2)	7744(2)	-1322(2)	13.3(5)
C6C	3072(2)	7823(2)	-435.4(19)	10.5(5)
C7C	4399(2)	10335.0(19)	1147.4(19)	9.0(5)
C8C	3201(2)	6988(2)	-258(2)	13.8(5)
O71C	5033.1(15)	10217.6(14)	1848.6(14)	11.3(4)
O72C	4392.1(16)	11103.6(14)	1143.5(14)	12.1(4)
O81C	3914.3(16)	7187.0(14)	594.3(14)	13.2(4)
O82C	2635(2)	6193.4(16)	-911.0(16)	24.8(5)
N1D	1239.3(18)	13848.8(17)	5109.4(17)	11.5(4)
C2D	2040(2)	14513(2)	5937(2)	13.2(5)
C3D	1897(2)	15141(2)	6711(2)	18.1(6)
C4D	883(3)	15080(2)	6603(2)	21.7(6)
C5D	44(2)	14408(2)	5738(2)	17.9(6)
C6D	260(2)	13794(2)	5004(2)	11.6(5)
C7D	3092(2)	14492(2)	5940(2)	14.0(5)
C8D	-559(2)	13008(2)	4036(2)	14.4(5)
O71D	3072.7(16)	13831.9(15)	5176.5(15)	15.7(4)
O72D	3893.1(17)	15090.9(16)	6662.6(17)	22.0(5)
O81D	-189.7(16)	12543.1(15)	3450.2(15)	14.8(4)
O82D	-1487.3(17)	12859.5(18)	3854.9(18)	25.4(5)
N1E	516.3(19)	12484.7(18)	2036.0(18)	13.8(5)
C2E	479(2)	13246(2)	1903(2)	17.7(6)
C3E	-91(3)	13169(3)	986(3)	24.3(7)
C4E	-619(3)	12278(3)	199(2)	26.1(7)
C5E	-578(3)	11487(3)	336(2)	21.5(7)
C6E	1(2)	11623(2)	1273(2)	15.2(6)

C7E	1093(3)	14173(2)	2832(2)	19.2(6)
C8E	96(2)	10825(2)	1519(2)	15.1(6)
O71E	1512.0(17)	14090.1(15)	3608.5(16)	17.7(4)
O72E	1149(2)	14927.9(19)	2815(2)	31.9(6)
O81E	774.5(16)	11078.9(15)	2411.0(15)	15.0(4)
O82E	-448.4(17)	10015.8(16)	911.0(16)	19.6(4)
N1F	3002.4(18)	11843.0(17)	4095.5(16)	10.7(4)
C2F	3723(2)	11850(2)	3785(2)	11.8(5)
C3F	4528(2)	11407(2)	3978(2)	15.2(6)
C4F	4573(3)	10933(2)	4504(2)	18.1(6)
C5F	3827(2)	10923(2)	4822(2)	15.7(6)
C6F	3056(2)	11399(2)	4608.9(19)	10.7(5)
C7F	3512(2)	12329(2)	3165(2)	11.5(5)
C8F	2213(2)	11471(2)	4931(2)	12.4(5)
O71F	2758.2(16)	12726.8(16)	3099.9(15)	15.7(4)
O72F	4054.3(16)	12287.9(15)	2741.0(14)	13.4(4)
O81F	1535.9(16)	11887.0(15)	4614.2(14)	13.3(4)
O82F	2235.2(17)	11135.5(16)	5468.5(16)	17.9(4)
O1W	2253.5(16)	11260.1(15)	871.6(15)	14.3(4)
O2W	3962(2)	14024.3(17)	2597.4(19)	28.2(6)
O3W	2189.7(19)	12976.7(18)	771.9(19)	24.8(5)
O4W	4179.5(17)	13467.0(15)	835.7(16)	17.3(4)
O5W	5538.8(16)	12997.1(15)	2200.6(15)	16.0(4)
O1S	2342.5(16)	10194.6(15)	1761.2(15)	16.1(4)
O2S	6466.0(18)	12083.4(16)	3208.8(16)	20.3(5)
O3S	2810.3(18)	13097.2(16)	-1053.0(16)	20.0(4)
O4S	705.4(19)	9381.6(18)	2546.5(18)	26.1(5)
O5S	5775.9(19)	14864.7(18)	1286.1(18)	25.4(5)
O6S	9420(2)	10614.2(19)	5909.2(19)	30.8(6)
O7S	1222(2)	11691(2)	6525(2)	32.0(6)
O8S	911(2)	12296(2)	-1196(2)	32.1(6)
O9S	1374(3)	7247(3)	3802(3)	52.3(8)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Ho-V. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	8.03(4)	8.03(5)	7.38(4)	4.35(4)	3.41(3)	3.14(3)
Ho1	11.74(6)	8.13(6)	9.29(5)	5.17(5)	6.38(4)	3.68(4)
U2	9.67(5)	11.26(5)	9.08(5)	4.39(4)	5.03(4)	3.67(4)
N1A	11.9(11)	11.4(11)	10.1(10)	5.4(9)	5.1(9)	3.3(9)
C2A	15.3(13)	17.0(14)	14.5(13)	9.1(12)	9.0(11)	6.8(11)
C3A	25.7(17)	32.9(19)	34.1(19)	23.9(17)	22.5(15)	14.2(15)
C4A	31.1(18)	29.7(19)	33.1(18)	25.5(16)	22.0(15)	13.6(15)
C5A	24.7(16)	18.4(15)	21.7(15)	15.8(13)	11.4(13)	10.6(13)
C6A	12.8(13)	12.0(13)	12.6(13)	6.4(11)	4.3(10)	3.2(10)
C7A	16.4(14)	18.7(15)	19.6(14)	12.7(12)	12.0(12)	10.1(11)

C8A	12.4(12)	10.8(13)	10.8(12)	4.7(11)	3.8(10)	3.5(10)
O71A	12.8(9)	15.5(10)	16.5(10)	10.2(9)	8.7(8)	7.9(8)
O72A	29.2(13)	43.1(16)	50.8(16)	36.1(14)	32.9(13)	27.0(12)
O81A	10.9(9)	13(1)	13.9(9)	8.2(8)	6.1(8)	5.9(8)
O82A	15.4(10)	13.5(10)	22.1(11)	10.7(9)	6.8(9)	7.6(8)
N1B	9(1)	10.0(11)	8.6(10)	5.3(9)	3.9(8)	4.0(8)
C2B	12.6(12)	11.7(13)	9.5(12)	7.1(10)	5.7(10)	5(1)
C3B	12.7(12)	14.0(13)	16.1(13)	10.8(11)	9.5(11)	5.8(10)
C4B	9.1(12)	14.8(14)	16.8(13)	9.2(12)	5.0(11)	3(1)
C5B	10.7(12)	14.9(14)	11.1(12)	6.6(11)	1.8(10)	1.4(10)
C6B	12.5(12)	13.7(13)	9.4(12)	7.3(11)	4.9(10)	5.2(10)
C7B	14.8(13)	10.1(13)	11.3(12)	7.6(11)	6.8(10)	5.3(10)
C8B	14.2(13)	12.0(13)	10.7(12)	6.0(11)	6.1(10)	3.8(10)
O71B	10.7(9)	14.2(10)	11.0(9)	5.4(8)	5.2(8)	3.3(8)
O72B	16.8(10)	12.3(10)	11.3(9)	7.2(8)	9.6(8)	6.5(8)
O81B	10.5(9)	14.8(10)	9.5(9)	5.3(8)	4.6(7)	3.6(8)
O82B	25.4(12)	21.6(12)	9.7(10)	0.6(9)	8.5(9)	-3.4(9)
N1C	9.8(10)	7.7(11)	8.3(10)	3.6(9)	3.9(8)	2.3(8)
C2C	9.8(12)	8.3(12)	9.4(12)	3.7(10)	3.5(10)	2.2(10)
C3C	17.6(14)	11.1(13)	14.2(13)	8.5(11)	4.8(11)	5.1(11)
C4C	16.6(14)	13.3(14)	12.5(13)	6.5(11)	3.7(11)	3.9(11)
C5C	15.0(13)	7.7(13)	10.0(12)	1.6(10)	2.3(10)	0.8(10)
C6C	12.3(12)	9.2(12)	9.5(12)	4.1(10)	5(1)	3.2(10)
C7C	9.2(11)	8.7(12)	9.8(12)	4.6(10)	4.9(10)	3.7(9)
C8C	17.7(14)	10.0(13)	11.9(13)	5.3(11)	5.3(11)	3.0(11)
O71C	12.4(9)	9.1(9)	9.8(9)	4.9(8)	2.5(7)	3.1(7)
O72C	14.2(9)	7.8(9)	13.5(9)	5.7(8)	5.2(8)	3.7(7)
O81C	16.9(10)	8.3(9)	10.4(9)	4.4(8)	3.1(8)	2.3(8)
O82C	34.0(13)	8.5(10)	14.4(11)	3.4(9)	-1.3(10)	-1.5(9)
N1D	10.7(11)	10.2(11)	13.2(11)	4.1(9)	6.7(9)	3.4(9)
C2D	13.3(13)	10.5(13)	14.3(13)	5.2(11)	5.9(11)	3.7(10)
C3D	18.5(14)	12.1(14)	14.2(14)	0.3(12)	5.9(12)	2.8(11)
C4D	24.7(16)	16.5(15)	20.3(15)	1.9(13)	14.7(13)	5.8(13)
C5D	17.8(14)	18.0(15)	22.3(15)	8.7(13)	14.0(12)	8.0(12)
C6D	12.9(13)	10.6(13)	13.0(13)	5.8(11)	7.3(10)	3.2(10)
C7D	10.7(12)	9.4(13)	17.5(14)	4.6(11)	4.6(11)	2.3(10)
C8D	11.8(13)	15.6(14)	15.3(13)	7.9(12)	5.3(11)	5.3(11)
O71D	11.4(9)	15.1(11)	18.1(10)	5.5(9)	7.3(8)	3.6(8)
O72D	12.8(10)	12.2(11)	24.9(12)	1.2(9)	3.1(9)	-0.2(8)
O81D	10.4(9)	15.9(11)	12.1(9)	3.3(8)	3.6(8)	2.7(8)
O82D	10.6(10)	26.7(13)	30.1(13)	6.5(11)	9.6(10)	2.3(9)
N1E	15.0(11)	16.9(13)	14.6(11)	9.7(10)	8.8(10)	8.8(10)
C2E	20.1(15)	21.5(16)	19.4(15)	12.5(13)	13.0(12)	10.7(12)
C3E	28.2(17)	32.0(19)	28.2(17)	23.3(16)	16.7(15)	15.6(15)
C4E	28.5(18)	40(2)	19.2(16)	20.6(16)	12.3(14)	16.4(16)
C5E	20.1(15)	33.1(19)	14.6(14)	13.6(14)	8.3(12)	10.6(14)
C6E	12.6(13)	21.7(15)	14.1(13)	9.8(12)	6.9(11)	8.4(11)
C7E	22.0(15)	18.2(15)	28.0(16)	14.2(14)	17.2(13)	11.6(12)

C8E	13.9(13)	19.4(15)	13.9(13)	7.1(12)	8.9(11)	8.8(11)
O71E	21.3(11)	13.9(11)	20.3(11)	8.2(9)	11.5(9)	7.2(9)
O72E	45.9(16)	22.6(13)	41.3(16)	20.4(12)	26.7(14)	15.1(12)
O81E	16.3(10)	15(1)	11.2(9)	5.7(8)	4.8(8)	6.1(8)
O82E	19.2(11)	16.4(11)	13.8(10)	2.5(9)	4.7(9)	1.7(9)
N1F	12.4(11)	11.3(11)	7.6(10)	3.3(9)	5.2(9)	2.7(9)
C2F	14.0(13)	12.7(13)	10.8(12)	5.7(11)	7.4(10)	4.9(10)
C3F	18.3(14)	19.3(15)	15.9(13)	10.2(12)	12.7(12)	9.3(12)
C4F	22.4(15)	23.5(16)	20.0(15)	15.3(13)	14.0(13)	16.0(13)
C5F	21.1(15)	17.6(15)	15.3(13)	11.2(12)	10.9(12)	8.7(12)
C6F	12.0(12)	12.6(13)	7.9(11)	4.4(10)	5.6(10)	2.2(10)
C7F	12.9(12)	11.6(13)	10.2(12)	5.5(11)	5.1(10)	2.9(10)
C8F	13.4(13)	12.4(13)	9.7(12)	3.5(11)	6.2(10)	1.2(10)
O71F	17.3(10)	21.9(11)	18.5(10)	14.3(9)	12.3(9)	10.3(9)
O72F	14(1)	18.9(11)	11.7(9)	8.7(8)	8.3(8)	5.1(8)
O81F	12.4(9)	17.8(11)	12.6(9)	8.6(8)	7.1(8)	4.3(8)
O82F	22.2(11)	22.7(12)	17.4(10)	13.3(9)	12.8(9)	7.0(9)
O1W	12.0(9)	18.4(11)	14.4(10)	10.3(9)	5.4(8)	2.1(8)
O2W	50.0(16)	18.4(12)	31.1(13)	11.8(11)	31.2(13)	16.4(11)
O3W	24.5(12)	28.1(13)	38.2(14)	22.9(12)	20.8(11)	16.1(10)
O4W	22.3(11)	13.3(10)	17.7(10)	9.9(9)	8.0(9)	2.7(9)
O5W	17(1)	8.9(10)	16.5(10)	5.0(8)	4.4(8)	-1.1(8)

Table 4 Bond Lengths for U-Ho-V.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	N1A	2.517(2)		O72B	Ho1[1]	2.3506(19)
U1	O71A	2.3960(19)		N1C	C2C	1.344(3)
U1	O81A	2.3657(19)		N1C	C6C	1.332(3)
U1	N1B	2.533(2)		C2C	C3C	1.380(4)
U1	O71B	2.3794(19)		C2C	C7C	1.506(4)
U1	O81B	2.316(2)		C3C	C4C	1.392(4)
U1	N1C	2.545(2)		C4C	C5C	1.386(4)
U1	O71C	2.4603(19)		C5C	C6C	1.389(4)
U1	O81C	2.393(2)		C6C	C8C	1.504(4)
Ho1	O72B[1]	2.3506(19)		C7C	O71C	1.277(3)
Ho1	O72C	2.3859(19)		C7C	O72C	1.242(3)
Ho1	O72F	2.3442(19)		C8C	O81C	1.285(3)
Ho1	O1W	2.383(2)		C8C	O82C	1.233(4)
Ho1	O2W	2.390(2)		N1D	C2D	1.333(4)
Ho1	O3W	2.351(2)		N1D	C6D	1.339(3)
Ho1	O4W	2.356(2)		C2D	C3D	1.385(4)
Ho1	O5W	2.341(2)		C2D	C7D	1.510(4)
U2	N1D	2.527(2)		C3D	C4D	1.387(4)
U2	O71D	2.384(2)		C4D	C5D	1.384(5)
U2	O81D	2.336(2)		C5D	C6D	1.390(4)
U2	N1E	2.536(2)		C6D	C8D	1.505(4)

U2	O71E	2.345(2)		C7D	O71D	1.276(4)
U2	O81E	2.432(2)		C7D	O72D	1.240(4)
U2	N1F	2.551(2)		C8D	O81D	1.291(3)
U2	O71F	2.390(2)		C8D	O82D	1.229(4)
U2	O81F	2.3783(19)		N1E	C2E	1.338(4)
N1A	C2A	1.339(4)		N1E	C6E	1.335(4)
N1A	C6A	1.337(4)		C2E	C3E	1.392(4)
C2A	C3A	1.387(4)		C2E	C7E	1.512(5)
C2A	C7A	1.508(4)		C3E	C4E	1.379(5)
C3A	C4A	1.389(5)		C4E	C5E	1.389(5)
C4A	C5A	1.387(4)		C5E	C6E	1.388(4)
C5A	C6A	1.388(4)		C6E	C8E	1.507(4)
C6A	C8A	1.511(4)		C7E	O71E	1.287(4)
C7A	O71A	1.285(3)		C7E	O72E	1.230(4)
C7A	O72A	1.225(3)		C8E	O81E	1.299(3)
C8A	O81A	1.299(3)		C8E	O82E	1.228(4)
C8A	O82A	1.227(3)		N1F	C2F	1.341(3)
N1B	C2B	1.340(3)		N1F	C6F	1.331(3)
N1B	C6B	1.333(4)		C2F	C3F	1.384(4)
C2B	C3B	1.388(4)		C2F	C7F	1.507(4)
C2B	C7B	1.500(4)		C3F	C4F	1.390(4)
C3B	C4B	1.391(4)		C4F	C5F	1.387(4)
C4B	C5B	1.389(4)		C5F	C6F	1.388(4)
C5B	C6B	1.390(4)		C6F	C8F	1.509(4)
C6B	C8B	1.515(4)		C7F	O71F	1.271(3)
C7B	O71B	1.266(3)		C7F	O72F	1.246(3)
C7B	O72B	1.255(3)		C8F	O81F	1.275(3)
C8B	O81B	1.296(3)		C8F	O82F	1.240(3)
C8B	O82B	1.220(3)				

[1]1-X,2-Y,-Z

II.26 U-Er-V

Table 1 Crystal data and structure refinement for U-Er-V.	
Identification code	U-Er-V
Empirical formula	$C_{84}H_{56}Er_2N_{12}O_{76}U_4$
Formula weight	3736.04
Temperature/K	99.99
Crystal system	triclinic
Space group	P-1
a/Å	14.3624(6)
b/Å	16.0902(7)
c/Å	17.1005(7)
α/°	115.045(2)

β/°	113.711(2)
γ/°	92.354(2)
Volume/Å^3	3169.9(2)
Z	1
ρ_{calc}g/cm^3	1.957
μ/mm^{-1}	6.508
F(000)	1756.0
Crystal size/mm^3	0.175 × 0.167 × 0.142
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.89 to 60.91
Index ranges	-20 ≤ h ≤ 20, -22 ≤ k ≤ 22, -24 ≤ l ≤ 24
Reflections collected	107853
Independent reflections	19088 [R_{int} = 0.0350, R_{sigma} = 0.0298]
Data/restraints/parameters	19088/0/762
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0238, wR_2 = 0.0534
Final R indexes [all data]	R_1 = 0.0304, wR_2 = 0.0554
Largest diff. peak/hole / e Å^{-3}	1.65/-1.57

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Er-V. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	5068.7(2)	8703.8(2)	1875.3(2)	7.57(2)
Er1	3702.4(2)	12461.2(2)	1362.2(2)	9.22(3)
U2	1558.9(2)	12703.2(2)	3736.3(2)	9.68(3)
N1A	4614.6(19)	7847.4(17)	2662.2(17)	10.6(4)
C2A	3785(2)	7947(2)	2839(2)	15.2(6)
C3A	3495(3)	7467(3)	3246(3)	23.8(7)
C4A	4085(3)	6868(3)	3478(3)	25.2(7)
C5A	4941(3)	6761(2)	3292(2)	19.2(6)
C6A	5181(2)	7268(2)	2885(2)	12.0(5)
C7A	3194(2)	8592(2)	2523(2)	14.5(6)
C8A	6072(2)	7196(2)	2620(2)	11.9(5)
O71A	3574.5(16)	8972.2(15)	2148.8(15)	13.2(4)
O72A	2396(2)	8701(2)	2616(2)	29.5(6)
O81A	6119.3(16)	7675.2(15)	2184.6(15)	12.1(4)
O82A	6666.2(17)	6702.9(15)	2807.2(16)	17.0(4)
N1B	6952.5(18)	9578.0(17)	2559.5(17)	9.3(4)
C2B	7416(2)	9389(2)	1983.7(19)	9.9(5)
C3B	8447(2)	9851(2)	2326(2)	12.2(5)
C4B	8999(2)	10539(2)	3304(2)	13.3(5)
C5B	8514(2)	10743(2)	3898(2)	13.7(5)
C6B	7486(2)	10237(2)	3498(2)	11.1(5)
C7B	6691(2)	8668(2)	939(2)	10.3(5)
C8B	6853(2)	10367(2)	4046(2)	12.8(5)
O71B	5756.2(16)	8362.7(15)	746.5(14)	12.4(4)
O72B	7043.1(16)	8447.3(14)	338.6(14)	11.2(4)
O81B	5916.2(15)	9804.9(15)	3518.0(14)	11.6(4)

O82B	7222.2(19)	10954.5(17)	4909.3(15)	21.9(5)
N1C	3692.7(18)	8653.4(16)	334.3(16)	8.9(4)
C2C	3627(2)	9444.8(19)	256.1(19)	9.4(5)
C3C	2922(2)	9431(2)	-591(2)	13.5(5)
C4C	2288(2)	8562(2)	-1398(2)	14.9(6)
C5C	2364(2)	7742(2)	-1323(2)	13.1(5)
C6C	3066(2)	7820(2)	-435(2)	10.6(5)
C7C	4398(2)	10337(2)	1149.1(19)	9.3(5)
C8C	3193(2)	6984(2)	-255(2)	13.3(5)
O71C	5032.8(16)	10219.4(14)	1849.8(14)	11.5(4)
O72C	4390.8(16)	11106.8(14)	1146.3(14)	11.7(4)
O81C	3912.5(16)	7185.5(14)	598.6(14)	13.5(4)
O82C	2632(2)	6192.4(16)	-908.8(16)	24.5(5)
N1D	1233.9(18)	13850.7(17)	5107.9(17)	10.6(4)
C2D	2037(2)	14511(2)	5939(2)	11.7(5)
C3D	1893(3)	15142(2)	6712(2)	18.5(6)
C4D	878(3)	15082(2)	6606(2)	20.4(6)
C5D	34(2)	14404(2)	5734(2)	16.2(6)
C6D	255(2)	13793(2)	5003(2)	11.6(5)
C7D	3091(2)	14496(2)	5946(2)	14.3(6)
C8D	-564(2)	13007(2)	4027(2)	13.4(5)
O71D	3070.4(16)	13836.0(15)	5176.7(15)	15.2(4)
O72D	3889.3(17)	15094.6(16)	6667.5(17)	21.9(5)
O81D	-189.7(16)	12544.0(15)	3444.8(15)	14.4(4)
O82D	-1488.2(17)	12858.9(17)	3846.7(18)	23.7(5)
N1E	517.3(19)	12490.5(18)	2031.2(18)	12.8(5)
C2E	482(3)	13255(2)	1903(2)	17.2(6)
C3E	-86(3)	13175(3)	986(3)	24.2(7)
C4E	-618(3)	12282(3)	193(2)	25.6(7)
C5E	-578(3)	11494(3)	332(2)	20.7(7)
C6E	2(2)	11626(2)	1268(2)	14.3(6)
C7E	1097(3)	14177(2)	2828(3)	19.8(6)
C8E	95(2)	10829(2)	1518(2)	12.7(5)
O71E	1513.6(18)	14096.3(16)	3606.9(16)	18.4(4)
O72E	1159(2)	14936.0(18)	2816(2)	31.5(6)
O81E	776.8(17)	11080.0(15)	2407.9(15)	14.5(4)
O82E	-448.8(18)	10019.6(16)	907.5(16)	19.7(5)
N1F	3004.3(19)	11846.2(17)	4092.9(16)	10.3(4)
C2F	3724(2)	11856(2)	3783.2(19)	10.4(5)
C3F	4532(2)	11413(2)	3980(2)	14.6(6)
C4F	4577(3)	10939(2)	4506(2)	17.7(6)
C5F	3829(2)	10927(2)	4823(2)	16.1(6)
C6F	3057(2)	11400(2)	4609.8(19)	10.9(5)
C7F	3513(2)	12334(2)	3165(2)	11.9(5)
C8F	2214(2)	11471(2)	4928.8(19)	11.6(5)
O71F	2758.2(17)	12730.8(15)	3097.9(15)	14.8(4)
O72F	4052.6(16)	12289.8(15)	2736.4(14)	13.2(4)
O81F	1537.6(16)	11888.8(15)	4611.7(14)	13.6(4)

O82F	2237.0(18)	11139.1(16)	5469.8(16)	18.2(4)
O1W	2261.1(16)	11263.7(15)	875.5(15)	14.1(4)
O2W	3953(2)	14016.0(17)	2583.1(19)	29.1(6)
O3W	2193.5(19)	12969.0(17)	769(2)	25.1(5)
O4W	4172.1(18)	13460.9(15)	831.9(16)	17.2(4)
O5W	5529.8(17)	12994.4(15)	2192.9(15)	16.2(4)
O1S	2341.0(17)	10193.8(15)	1762.0(15)	15.7(4)
O2S	6465.3(18)	12087.6(16)	3211.3(16)	19.3(5)
O3S	2812.7(18)	13092.0(16)	-1055.0(17)	20.7(5)
O4S	707(2)	9382.1(18)	2546.2(18)	26.4(5)
O5S	5778(2)	14860.0(18)	1283.9(18)	25.9(5)
O6S	9420(2)	10615.3(19)	5908.9(19)	30.2(6)
O7S	1222(2)	11696(2)	6522(2)	32.5(6)
O8S	908(2)	12291(2)	-1201(2)	32.6(6)
O9S	1376(3)	7238(2)	3807(2)	48.2(8)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Er-V. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	7.79(5)	8.23(5)	6.99(4)	4.10(4)	3.15(4)	2.70(4)
Er1	12.07(6)	8.40(6)	9.27(5)	4.78(5)	6.17(5)	2.94(4)
U2	9.13(5)	10.79(5)	8.28(5)	3.41(4)	4.51(4)	2.83(4)
N1A	12.2(11)	10.3(11)	10.2(11)	5.4(9)	5.3(9)	3.9(9)
C2A	18.3(15)	16.6(15)	16.9(14)	10.0(12)	11.3(12)	8.5(12)
C3A	27.9(18)	31.8(19)	32.6(18)	23.9(16)	23.0(16)	14.7(15)
C4A	29.3(19)	33(2)	34.4(19)	26.2(17)	21.9(16)	13.6(16)
C5A	25.5(17)	17.4(15)	21.9(15)	13.9(13)	12.3(14)	9.7(13)
C6A	11.4(13)	12.2(13)	9.8(12)	4.8(11)	3.3(10)	2.1(11)
C7A	13.7(14)	17.9(15)	17.4(14)	10.7(12)	9.3(12)	7.9(12)
C8A	11.2(13)	10.5(13)	10.5(12)	4.2(11)	3.1(10)	3(1)
O71A	13.6(10)	14.9(10)	16.2(10)	9.6(9)	8.6(8)	7.2(8)
O72A	28.4(14)	41.4(16)	50.5(17)	34.6(14)	31.5(13)	24.3(12)
O81A	11.3(10)	14.6(10)	14.1(10)	9.2(8)	6.5(8)	6.5(8)
O82A	15.5(11)	15.9(11)	21.3(11)	11.8(9)	6.6(9)	8.6(9)
N1B	9.7(11)	10.1(11)	9.2(10)	5.3(9)	4.5(9)	3.7(9)
C2B	11.5(13)	10.7(13)	9.2(12)	5.3(10)	5.5(10)	4.7(10)
C3B	12.2(13)	15.4(14)	16.9(13)	11.5(12)	9.4(11)	6.8(11)
C4B	8.6(13)	13.6(14)	16.5(14)	8.5(12)	3.5(11)	1.4(11)
C5B	13.8(14)	13.2(14)	11.6(13)	6.0(11)	3.6(11)	3.0(11)
C6B	10.9(13)	14.3(14)	9.2(12)	7.6(11)	3.5(10)	4.1(11)
C7B	11.0(13)	11.9(13)	12.7(12)	8.8(11)	6.3(11)	6.3(10)
C8B	13.7(14)	15.2(14)	11.4(12)	8.1(11)	5.8(11)	2.9(11)
O71B	11.6(10)	14.5(10)	10.3(9)	4.9(8)	5.7(8)	2.9(8)
O72B	14.1(10)	12.2(10)	11.8(9)	6.9(8)	8.6(8)	5.4(8)
O81B	9.6(9)	14.9(10)	10.5(9)	5.4(8)	5.5(8)	3.0(8)
O82B	25.1(12)	22.6(12)	9.3(10)	0.9(9)	8.5(9)	-3.6(10)

N1C	10.2(11)	7.3(11)	8(1)	3.1(9)	3.7(9)	2.0(9)
C2C	9.6(12)	8.1(12)	9.9(12)	3.8(10)	4.6(10)	1.5(10)
C3C	16.4(14)	9.9(13)	13.3(13)	7.3(11)	4.2(11)	3.4(11)
C4C	14.7(14)	14.4(14)	9.4(13)	5.9(11)	0.1(11)	3.5(11)
C5C	12.5(13)	10.5(13)	9.0(12)	2.3(11)	1.2(11)	1.1(11)
C6C	10.9(13)	9.3(13)	9.2(12)	3.8(10)	3.3(10)	2.8(10)
C7C	9.5(12)	9.8(12)	9.8(12)	4.5(10)	5.6(10)	2(1)
C8C	16.1(14)	10.6(13)	11.6(13)	5.1(11)	5.4(11)	2.0(11)
O71C	12.2(10)	9.4(9)	10.2(9)	4.9(8)	2.6(8)	2.2(8)
O72C	13.2(10)	6.7(9)	12.5(9)	4.6(8)	3.7(8)	1.6(8)
O81C	16.6(10)	9.5(10)	10.6(9)	4.9(8)	3.0(8)	2.6(8)
O82C	34.5(14)	8.9(10)	13.4(11)	3.3(9)	-0.8(10)	-2.2(10)
N1D	9.5(11)	10.3(11)	10.6(11)	3.9(9)	4.6(9)	2.4(9)
C2D	9.2(13)	9.2(13)	11.9(13)	3.0(11)	3(1)	1.6(10)
C3D	17.5(15)	13.6(14)	14.6(14)	0.3(12)	5.7(12)	2.7(12)
C4D	22.5(16)	16.4(15)	18.8(15)	2.3(13)	12.7(13)	6.6(13)
C5D	14.7(14)	15.8(15)	18.8(14)	6.0(12)	10.8(12)	4.5(12)
C6D	12.4(13)	10.5(13)	13.9(13)	6.5(11)	7.3(11)	3.2(11)
C7D	12.6(14)	9.5(13)	16.8(14)	4.9(11)	5.0(11)	1.6(11)
C8D	11.2(13)	12.3(14)	14.5(13)	6.1(11)	4.3(11)	2.8(11)
O71D	11.1(10)	13.1(10)	17(1)	3.3(9)	6.8(8)	2.5(8)
O72D	11.4(10)	12.8(11)	23.9(12)	0.9(9)	1.5(9)	-2.0(8)
O81D	10.1(10)	16.4(10)	10.7(9)	2.9(8)	3.5(8)	2.6(8)
O82D	9.5(10)	26.1(13)	25.5(12)	5.5(10)	6.9(9)	1.3(9)
N1E	12.0(12)	17.0(12)	13.8(11)	8.7(10)	8(1)	7.4(10)
C2E	20.0(16)	19.1(15)	20.2(15)	11.8(13)	13.0(13)	9.5(13)
C3E	27.8(18)	34(2)	27.3(17)	23.5(16)	16.9(15)	16.7(15)
C4E	27.5(18)	39(2)	18.6(16)	19.7(16)	11.5(14)	15.0(16)
C5E	19.3(16)	29.1(18)	12.8(14)	9.4(13)	7.3(12)	7.9(14)
C6E	12.9(14)	18.4(15)	13.9(13)	8.0(12)	7.8(11)	6.4(11)
C7E	20.5(16)	21.1(16)	28.7(17)	15.2(14)	17.0(14)	10.5(13)
C8E	9.8(13)	17.3(14)	10.2(12)	5.2(11)	5.3(10)	5.7(11)
O71E	21.9(12)	15.5(11)	18.6(11)	7.5(9)	10.5(9)	7.3(9)
O72E	44.2(17)	22.2(13)	40.7(16)	20.7(12)	24.2(14)	13.8(12)
O81E	15.5(10)	14.5(10)	11.0(9)	5.7(8)	4.4(8)	5.5(8)
O82E	18.7(11)	17.2(11)	15.1(10)	3.1(9)	5.8(9)	2.4(9)
N1F	10.9(11)	9.9(11)	7.4(10)	3.4(9)	3.0(9)	1.1(9)
C2F	12.7(13)	10.9(13)	6.3(11)	2.6(10)	5.1(10)	1.8(10)
C3F	16.5(14)	19.6(15)	13.1(13)	9.2(12)	9.8(12)	8.5(12)
C4F	22.5(16)	22.1(16)	18.9(15)	13.4(13)	14.1(13)	13.8(13)
C5F	19.8(15)	18.8(15)	16.2(14)	11.4(12)	10.7(12)	8.2(12)
C6F	11.2(13)	12.5(13)	6.9(11)	3.3(10)	3.9(10)	1.9(10)
C7F	14.0(13)	12.8(13)	9.4(12)	5.1(11)	6.1(11)	2.9(11)
C8F	10.6(13)	13.2(13)	7.5(12)	3.6(11)	3(1)	-1.2(11)
O71F	16.8(11)	19.5(11)	16.5(10)	12.4(9)	10.7(9)	9.4(9)
O72F	12.3(10)	18.6(11)	11.1(9)	7.8(8)	6.9(8)	3.2(8)
O81F	11.4(10)	18.4(11)	11.7(9)	7.6(8)	5.7(8)	3.5(8)
O82F	21.7(11)	24.5(12)	17.4(10)	13.8(10)	13.0(9)	7.7(9)

O1W	12.8(10)	16.2(11)	15.3(10)	9.9(9)	6.0(8)	2.5(8)
O2W	52.9(17)	16.4(12)	33.1(14)	11.3(11)	33.2(14)	16.1(12)
O3W	25.5(13)	26.3(13)	41.7(15)	23.7(12)	22.8(12)	15.8(11)
O4W	21.0(11)	15.8(11)	18.0(11)	11.4(9)	8.4(9)	3.9(9)
O5W	15.7(11)	10.6(10)	15(1)	4.7(8)	2.6(8)	-1.8(8)

Table 4 Bond Lengths for U-Er-V.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	N1A	2.517(2)		O72B	Er1[1]	2.347(2)
U1	O71A	2.392(2)		N1C	C2C	1.339(3)
U1	O81A	2.366(2)		N1C	C6C	1.340(3)
U1	N1B	2.533(2)		C2C	C3C	1.384(4)
U1	O71B	2.3837(19)		C2C	C7C	1.508(4)
U1	O81B	2.317(2)		C3C	C4C	1.393(4)
U1	N1C	2.544(2)		C4C	C5C	1.383(4)
U1	O71C	2.4596(19)		C5C	C6C	1.391(4)
U1	O81C	2.393(2)		C6C	C8C	1.503(4)
Er1	O72B[1]	2.347(2)		C7C	O71C	1.277(3)
Er1	O72C	2.377(2)		C7C	O72C	1.241(3)
Er1	O72F	2.3367(19)		C8C	O81C	1.290(3)
Er1	O1W	2.371(2)		C8C	O82C	1.228(4)
Er1	O2W	2.376(2)		N1D	C2D	1.335(4)
Er1	O3W	2.339(2)		N1D	C6D	1.338(4)
Er1	O4W	2.346(2)		C2D	C3D	1.387(4)
Er1	O5W	2.330(2)		C2D	C7D	1.510(4)
U2	N1D	2.532(2)		C3D	C4D	1.388(5)
U2	O71D	2.382(2)		C4D	C5D	1.394(4)
U2	O81D	2.335(2)		C5D	C6D	1.391(4)
U2	N1E	2.542(2)		C6D	C8D	1.510(4)
U2	O71E	2.345(2)		C7D	O71D	1.282(4)
U2	O81E	2.435(2)		C7D	O72D	1.237(4)
U2	N1F	2.552(2)		C8D	O81D	1.293(4)
U2	O71F	2.389(2)		C8D	O82D	1.223(4)
U2	O81F	2.378(2)		N1E	C2E	1.336(4)
N1A	C2A	1.343(4)		N1E	C6E	1.337(4)
N1A	C6A	1.338(4)		C2E	C3E	1.391(4)
C2A	C3A	1.384(4)		C2E	C7E	1.505(5)
C2A	C7A	1.506(4)		C3E	C4E	1.383(5)
C3A	C4A	1.387(5)		C4E	C5E	1.384(5)
C4A	C5A	1.388(5)		C5E	C6E	1.388(4)
C5A	C6A	1.385(4)		C6E	C8E	1.510(4)
C6A	C8A	1.514(4)		C7E	O71E	1.290(4)
C7A	O71A	1.291(3)		C7E	O72E	1.229(4)
C7A	O72A	1.228(4)		C8E	O81E	1.298(3)
C8A	O81A	1.294(3)		C8E	O82E	1.227(4)
C8A	O82A	1.230(3)		N1F	C2F	1.340(3)

N1B	C2B	1.340(3)		N1F	C6F	1.338(3)
N1B	C6B	1.338(4)		C2F	C3F	1.387(4)
C2B	C3B	1.389(4)		C2F	C7F	1.500(4)
C2B	C7B	1.507(4)		C3F	C4F	1.391(4)
C3B	C4B	1.395(4)		C4F	C5F	1.388(4)
C4B	C5B	1.390(4)		C5F	C6F	1.385(4)
C5B	C6B	1.389(4)		C6F	C8F	1.506(4)
C6B	C8B	1.511(4)		C7F	O71F	1.271(4)
C7B	O71B	1.267(3)		C7F	O72F	1.248(3)
C7B	O72B	1.249(3)		C8F	O81F	1.276(3)
C8B	O81B	1.294(3)		C8F	O82F	1.240(3)
C8B	O82B	1.226(4)				

[1]1-X,2-Y,-Z

II.27 U-Lu-VI

Table 1 Crystal data and structure refinement for U-Lu-VI.	
Identification code	U-Lu-VI
Empirical formula	$C_{56}H_{42}Lu_2N_8O_{62}U_2$
Formula weight	2644.97
Temperature/K	99.99
Crystal system	triclinic
Space group	P-1
a/Å	13.0826(5)
b/Å	13.1980(5)
c/Å	14.3851(6)
α/°	113.484(2)
β/°	97.098(2)
γ/°	98.492(2)
Volume/Å^3	2207.06(15)
Z	1
ρ_{calc}g/cm^3	1.990
μ/mm^{-1}	5.992
F(000)	1256.0
Crystal size/mm^3	0.225 × 0.206 × 0.106
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.152 to 52.744
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -17 ≤ l ≤ 17
Reflections collected	53645
Independent reflections	8944 [R_{int} = 0.0336, R_{sigma} = 0.0271]
Data/restraints/parameters	8944/0/551
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0293, wR_2 = 0.0676
Final R indexes [all data]	R_1 = 0.0360, wR_2 = 0.0709

Largest diff. peak/hole / e Å^{-3}	3.72/-0.82

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Lu-VI. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	1753.4(2)	6815.7(2)	3296.6(2)	7.58(5)
Lu0A	4457.4(2)	2432.2(2)	-1154.0(2)	6.96(6)
O81A	779(3)	7547(3)	2350(3)	13.5(7)
O71D	3648(3)	459(3)	-1790(3)	10.6(7)
O81D	4037(3)	3833(3)	-1583(3)	11.2(7)
O71A	3275(3)	7878(3)	4648(3)	12.2(7)
O1W	3060(3)	2366(3)	-369(3)	13.8(7)
O71B	3112(3)	7085(3)	2332(2)	11.6(7)
O81B	199(3)	5369(3)	2626(3)	13.3(7)
O81C	2708(3)	5390(3)	3249(3)	13.2(7)
O4W	5054(3)	1542(3)	-2637(3)	16.6(8)
O2W	4860(3)	3956(3)	468(2)	12.6(7)
O71C	732(3)	7625(3)	4502(3)	11.0(7)
O3W	5468(3)	1820(3)	-172(3)	16.0(7)
N1B	1501(3)	5382(3)	1417(3)	9.0(8)
N1A	2283(3)	8949(3)	3819(3)	9.5(8)
N1C	1617(3)	6080(3)	4673(3)	9.2(8)
C2B	2210(4)	5459(4)	843(4)	9.1(9)
C8A	846(4)	8569(4)	2451(4)	13.3(10)
C2C	993(4)	6470(4)	5363(4)	9.4(9)
O72C	-147(3)	7763(3)	5768(3)	14.4(7)
O82A	289(3)	8884(3)	1918(3)	21.2(8)
C3C	876(4)	6062(4)	6100(4)	12.1(10)
N1D	2905(3)	1794(3)	-2509(3)	7.6(8)
C6B	644(4)	4531(4)	996(4)	9.9(9)
C7C	467(4)	7353(4)	5218(4)	9.9(9)
O72A	4359(3)	9445(3)	5862(3)	14.0(7)
O72B	3887(3)	6501(3)	966(2)	11.4(7)
O82B	-916(3)	3806(3)	1416(3)	16.7(8)
C4A	2806(4)	11249(4)	4394(4)	15.5(11)
C6D	2567(4)	2536(4)	-2812(4)	9.6(9)
C7B	3143(4)	6420(4)	1408(4)	9.4(9)
C7A	3630(4)	8945(4)	5090(4)	10.8(10)
C2A	3094(4)	9603(4)	4606(4)	10.5(9)
C6C	2147(4)	5310(4)	4726(4)	10.3(9)
O72D	2382(3)	-1039(3)	-2903(3)	13.7(7)
O82D	3044(3)	4448(3)	-2543(3)	18.1(8)
O82C	3451(3)	4377(4)	3948(3)	29.5(10)
C3D	1377(4)	385(4)	-3597(4)	12.6(10)
C5B	469(4)	3728(4)	-17(4)	13.1(10)
C7D	2828(4)	4(4)	-2490(4)	10.2(9)
C4C	1418(4)	5247(4)	6139(4)	13.1(10)
C3A	3385(4)	10765(4)	4915(4)	13.3(10)

C4B	1200(4)	3818(4)	-619(4)	14.9(10)
C2D	2334(4)	733(4)	-2895(4)	10.8(9)
C8B	-105(4)	4547(4)	1719(4)	11(1)
C5D	1623(4)	2254(4)	-3517(4)	12.6(10)
C5C	2076(4)	4868(4)	5443(4)	13.2(10)
C5A	1951(4)	10570(4)	3581(4)	14.5(10)
C8D	3268(4)	3705(4)	-2292(4)	11.9(10)
C4D	1024(4)	1162(4)	-3907(4)	14.2(10)
C8C	2826(4)	4971(4)	3919(4)	15.9(10)
C6A	1730(4)	9419(4)	3316(4)	12.4(10)
C3B	2091(4)	4700(4)	-183(4)	11.4(10)
O5S	-1392(3)	9275(3)	870(3)	19.7(8)
O3S	3030(3)	6624(3)	-1513(3)	18.7(8)
O4S	3470(3)	3763(3)	1664(3)	21.0(8)
O1S	5044(3)	7888(3)	6473(3)	24.5(9)
O8S	1374(3)	10730(3)	1055(3)	26.2(9)
O9S	102(4)	8367(4)	7895(4)	34.9(10)
O2S	5446(4)	6275(4)	4705(4)	36.4(11)
O6SB	3337(7)	7541(9)	7150(10)	17(3)
O7SB	1570(12)	8598(11)	-258(15)	43(5)
O11S	3656(3)	9859(3)	22(3)	20.8(8)
O10S	3495(3)	1734(3)	1785(3)	24.9(9)
O6SA	3550(9)	7876(11)	7579(12)	20(3)
O7SA	1780(6)	8549(6)	200(8)	28(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U-Lu-VI. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	7.31(9)	7.58(9)	5.45(9)	1.31(7)	1.34(6)	-1.21(6)
Lu0A	5.9(1)	6.03(10)	6.9(1)	1.48(8)	1.00(7)	-0.86(7)
O81A	13.6(17)	12.0(17)	10.9(17)	2.8(14)	-0.9(14)	-0.1(14)
O71D	8.3(15)	8.2(16)	13.7(17)	4.3(13)	0.4(14)	-0.8(13)
O81D	10.3(16)	8.3(16)	11.2(16)	2.4(13)	0.4(14)	-2.5(13)
O71A	14.1(17)	6.9(16)	12.8(17)	2.9(14)	0.4(14)	-0.6(13)
O1W	12.7(17)	12.9(17)	10.7(17)	0.6(14)	4.8(14)	-1.3(14)
O71B	11.7(16)	11.8(16)	6.7(16)	0.2(13)	4.6(13)	-2.6(13)
O81B	13.1(17)	12.2(17)	9.8(16)	0.8(14)	5.9(14)	-2.7(13)
O81C	15.3(17)	15.9(17)	8.9(16)	4.8(14)	6.8(14)	2.6(14)
O4W	10.8(17)	11.1(17)	15.5(18)	-4.2(14)	3.5(14)	-6.2(14)
O2W	14.7(17)	8.4(16)	9.0(16)	-1.4(13)	6.4(14)	-2.8(13)
O71C	12.9(16)	11.4(16)	10.1(16)	5.1(14)	4.7(14)	2.9(13)
O3W	13.9(17)	10.7(17)	20.5(19)	6.1(15)	-3.6(15)	1.0(14)
N1B	6.0(18)	12(2)	8.3(19)	5.1(16)	-0.2(15)	0.6(15)
N1A	9.7(19)	11.2(19)	6.7(18)	1.5(16)	5.0(16)	2.7(15)
N1C	7.2(18)	9.5(19)	8.2(19)	1.6(16)	2.9(15)	-1.1(15)
C2B	10(2)	6(2)	12(2)	4.1(18)	3.0(19)	0.6(17)

C8A	10(2)	17(3)	17(2)	10(2)	5(2)	3.9(19)
C2C	7(2)	7(2)	8(2)	-0.8(18)	0.1(18)	-2.8(17)
O72C	14.4(17)	14.0(17)	15.6(18)	5.0(14)	7.5(15)	5.2(14)
O82A	21.6(19)	18.8(19)	22(2)	11.1(16)	-6.7(17)	3.6(16)
C3C	11(2)	15(2)	9(2)	4.3(19)	2.9(19)	0.7(19)
N1D	8.4(18)	5.8(18)	6.5(18)	0.5(15)	2.1(15)	0.4(15)
C6B	7(2)	6(2)	13(2)	1.4(18)	4.5(19)	-2.2(17)
C7C	5(2)	9(2)	8(2)	-1.6(18)	-0.4(18)	-3.5(17)
O72A	11.3(16)	11.5(17)	10.0(17)	-1.1(14)	-4.8(14)	-2.3(13)
O72B	10.7(16)	11.7(16)	8.8(16)	2.2(13)	3.4(13)	-1.1(13)
O82B	11.8(17)	14.2(17)	17.5(18)	2.3(15)	5.2(15)	-5.0(14)
C4A	16(2)	9(2)	19(3)	3(2)	9(2)	2.6(19)
C6D	11(2)	10(2)	6(2)	1.6(18)	3.1(18)	2.7(18)
C7B	9(2)	11(2)	10(2)	5.0(19)	2.8(19)	2.7(18)
C7A	11(2)	11(2)	9(2)	2.2(19)	5.8(19)	1.0(18)
C2A	8(2)	12(2)	9(2)	1.5(19)	3.0(18)	1.6(18)
C6C	9(2)	9(2)	11(2)	2.7(19)	2.3(19)	1.7(18)
O72D	11.9(17)	6.9(16)	19.1(18)	4.4(14)	-2.7(15)	0.2(13)
O82D	22.7(19)	8.5(17)	21.4(19)	7.4(15)	-1.8(16)	0.2(14)
O82C	37(2)	45(3)	26(2)	23(2)	19(2)	32(2)
C3D	10(2)	10(2)	14(2)	2.3(19)	-0.3(19)	-0.7(18)
C5B	10(2)	10(2)	13(2)	0.2(19)	0.5(19)	-2.2(18)
C7D	9(2)	10(2)	11(2)	2.1(19)	5.9(19)	1.5(18)
C4C	14(2)	14(2)	10(2)	5(2)	2.7(19)	-0.7(19)
C3A	11(2)	11(2)	13(2)	1.3(19)	1.7(19)	-2.2(19)
C4B	14(2)	13(2)	11(2)	-1(2)	4(2)	0(2)
C2D	9(2)	12(2)	10(2)	3.3(19)	0.5(18)	0.3(18)
C8B	13(2)	13(2)	8(2)	6.2(19)	1.1(19)	2.0(19)
C5D	14(2)	12(2)	13(2)	6(2)	0(2)	4.7(19)
C5C	13(2)	15(2)	14(2)	8(2)	3(2)	5.9(19)
C5A	17(3)	13(2)	15(2)	7(2)	3(2)	5(2)
C8D	14(2)	11(2)	9(2)	3.1(19)	3.8(19)	2.1(19)
C4D	10(2)	14(2)	13(2)	2(2)	-3(2)	-0.2(19)
C8C	13(2)	19(3)	17(3)	7(2)	3(2)	7(2)
C6A	13(2)	14(2)	10(2)	4.3(19)	6(2)	2.0(19)
C3B	7(2)	17(2)	9(2)	5(2)	4.9(18)	0.2(19)
O5S	13.3(18)	23(2)	23(2)	11.0(17)	2.6(16)	-0.2(15)

Table 4 Bond Lengths for U-Lu-VI.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O81A	2.322(4)		C8A	O82A	1.223(6)
U1	O71A	2.399(3)		C8A	C6A	1.514(7)
U1	O71B	2.454(3)		C2C	C3C	1.381(7)
U1	O81B	2.369(3)		C2C	C7C	1.507(7)
U1	O81C	2.392(3)		O72C	C7C	1.228(6)
U1	O71C	2.335(3)		C3C	C4C	1.387(7)

U1	N1B	2.553(4)		N1D	C6D	1.329(6)
U1	N1A	2.565(4)		N1D	C2D	1.341(6)
U1	N1C	2.543(4)		C6B	C5B	1.384(7)
Lu0A	O71D	2.406(3)		C6B	C8B	1.511(6)
Lu0A	O81D	2.286(3)		O72A	C7A	1.244(6)
Lu0A	O1W	2.273(3)		O72B	Lu0A[1]	2.323(3)
Lu0A	O4W	2.286(3)		O72B	C7B	1.241(5)
Lu0A	O2W	2.326(3)		O82B	C8B	1.230(6)
Lu0A	O3W	2.272(4)		C4A	C3A	1.389(7)
Lu0A	N1D	2.417(4)		C4A	C5A	1.402(7)
Lu0A	O72B[1]	2.323(3)		C6D	C5D	1.396(7)
O81A	C8A	1.286(6)		C6D	C8D	1.508(6)
O71D	C7D	1.259(6)		C7A	C2A	1.506(7)
O81D	C8D	1.281(6)		C2A	C3A	1.393(7)
O71A	C7A	1.274(6)		C6C	C5C	1.379(7)
O71B	C7B	1.279(6)		C6C	C8C	1.515(7)
O81B	C8B	1.285(6)		O72D	C7D	1.271(6)
O81C	C8C	1.293(6)		O82D	C8D	1.232(6)
O71C	C7C	1.288(6)		O82C	C8C	1.221(6)
N1B	C2B	1.334(6)		C3D	C2D	1.395(7)
N1B	C6B	1.343(6)		C3D	C4D	1.385(7)
N1A	C2A	1.345(6)		C5B	C4B	1.390(7)
N1A	C6A	1.338(7)		C7D	C2D	1.490(7)
N1C	C2C	1.354(6)		C4C	C5C	1.391(7)
N1C	C6C	1.332(6)		C4B	C3B	1.394(7)
C2B	C7B	1.495(6)		C5D	C4D	1.386(7)
C2B	C3B	1.387(6)		C5A	C6A	1.385(7)

[1]1-X,1-Y,-Z

II.28 $(UO_2)_5(dpa)_8(Gd)_2(H_2O)_{12};10H_2O$

Table 1 Crystal data and structure refinement for (UO2)5(dpa)8(Gd)2(H2O)12;10H2O.	
Identification code	(UO2)5(dpa)8(Gd)2(H2O)12;10H2O
Empirical formula	$C_{56}H_{48}Gd_2N_8O_{64}U_5$
Formula weight	3361.67
Temperature/K	300.31
Crystal system	triclinic
Space group	P-1
a/Å	8.6966(6)
b/Å	13.0542(9)
c/Å	19.4264(13)
α/°	88.293(4)
β/°	88.655(3)
γ/°	83.203(4)

Volume/Å^3	2188.5(3)
Z	1
ρ_{calc}g/cm^3	2.551
μ/mm^{-1}	10.830
F(000)	1540.0
Crystal size/mm^3	0.278 × 0.141 × 0.105
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.144 to 61.012
Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -27 ≤ l ≤ 27
Reflections collected	70513
Independent reflections	13246 [R_{int} = 0.0366, R_{sigma} = 0.0288]
Data/restraints/parameters	13246/0/616
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0222, wR_2 = 0.0506
Final R indexes [all data]	R_1 = 0.0299, wR_2 = 0.0531
Largest diff. peak/hole / e Å^{-3}	1.23/-0.74

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for (UO2)5(dpa)8(Gd)2(H2O)12;10H2O. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	0	0	5000	21.27(4)
U3	2647.5(2)	-1197.9(2)	-2343.3(2)	23.47(3)
U2	2728.2(2)	2463.1(2)	2.7(2)	23.01(3)
Gd1	6475.2(2)	2781.5(2)	-2696.7(2)	25.53(4)
O81C	4368(3)	2872(2)	-992.7(13)	38.2(6)
O6AA	7459(3)	1095.4(19)	-3009.0(13)	34.3(6)
N1C	5070(3)	3488(2)	174.3(13)	21.9(5)
O81A	1386(3)	-929.8(19)	4040.5(13)	36.9(6)
O5W	9165(3)	2542(2)	-2387.0(14)	39.3(6)
N1A	1258(3)	1054(2)	3996.5(15)	26.3(6)
O71D	3823(3)	-8.8(19)	-3068.0(12)	32.5(5)
O4W	7738(4)	3033(2)	-3800.7(14)	44.0(7)
O2W	4663(3)	2389(2)	-3548.3(15)	44.2(7)
N1D	3846(3)	-1904(2)	-3437.6(14)	25.3(6)
O22Y	1431(3)	3511.3(19)	-316.9(13)	32.8(5)
O71C	2854(3)	3365(2)	1057.6(13)	35.8(6)
O6W	7049(4)	4517(2)	-2804.3(16)	51.3(8)
O82C	6597(3)	3190(2)	-1499.9(13)	34.7(6)
N1B	390(3)	1411(2)	-278.8(14)	22.8(5)
O11Y	1696(3)	-152(2)	5476.1(15)	43.6(7)
O81D	2469(3)	-2974(2)	-2524.2(14)	40.5(6)
O72B	1927(3)	421(2)	-1827.1(14)	44.4(7)
O32Y	926(3)	-906(2)	-2797.7(15)	43.2(7)
O21Y	3985(3)	1393(2)	305.5(15)	37.8(6)
O1W	5044(3)	1528(2)	-2114.7(14)	41.2(7)
O71B	2755(3)	1451(2)	-1072.9(15)	48.7(8)
O81B	810(3)	2138(2)	908.9(13)	39.9(6)
C8C	5690(4)	3185(3)	-997.6(17)	26.0(7)

O31Y	4409(3)	-1473(2)	-1908.7(14)	42.6(7)
O3W	4047(3)	3848(2)	-2476.7(16)	47.0(7)
O19	1420(4)	-1709(3)	-1329.5(16)	53.2(8)
O72D	4966(3)	456(2)	-4047.9(13)	33.5(6)
C2C	5341(4)	3806(2)	805.4(17)	25.1(6)
C6B	-804(4)	1410(3)	160.6(18)	26.2(7)
O72C	4085(3)	4062(2)	1895.1(13)	42.4(7)
C5C	7550(4)	3922(3)	-201.2(18)	28.0(7)
C6C	6148(4)	3562(2)	-319.4(16)	23.5(6)
C7D	4434(4)	-185(3)	-3667.5(17)	25.9(7)
C3C	6712(4)	4173(3)	968.5(19)	31.6(7)
C7C	4003(4)	3751(3)	1308.7(18)	29.9(7)
C6D	3785(4)	-2893(3)	-3588.8(19)	32.3(8)
C4C	7836(4)	4221(3)	456(2)	32.7(8)
C2B	269(4)	1023(3)	-903.8(17)	26.1(7)
C6A	1915(4)	581(3)	3446.8(17)	25.0(6)
O82D	2828(4)	-4408(2)	-3133.3(17)	53.8(8)
C5B	-2186(4)	1074(3)	-17(2)	33.3(8)
C8A	1956(4)	-571(3)	3498.2(18)	26.6(7)
C2A	1154(4)	2081(3)	4000(2)	36.7(9)
C8D	2982(5)	-3491(3)	-3043(2)	36.4(8)
C3B	-1084(4)	686(3)	-1126(2)	33.3(8)
C4B	-2340(4)	729(3)	-673(2)	36.5(8)
C5A	2486(4)	1096(3)	2883.3(18)	31.2(7)
C7B	1748(4)	969(3)	-1304.8(18)	31.2(8)
C2D	4480(4)	-1283(3)	-3891.1(17)	26.4(7)
C4A	2363(4)	2161(3)	2890(2)	40.8(9)
C3D	5089(5)	-1633(3)	-4513.7(19)	38.1(9)
C3A	1677(5)	2662(3)	3452(3)	47.3(11)
C5D	4384(6)	-3298(3)	-4198(2)	48.8(11)
C8B	-444(4)	1781(3)	852.6(19)	32.8(8)
O71A	32(5)	1893(2)	5089.1(18)	68.9(12)
C4D	5040(6)	-2660(4)	-4669(2)	53.8(12)
C7A	450(7)	2538(3)	4645(3)	65.8(16)
O72A	375(7)	3478(3)	4719(3)	124(2)
O1S	969(4)	3891(3)	-1796.9(17)	55.8(8)
O2S	90(4)	4040(2)	1905.8(17)	51.0(8)
O4S	1364(5)	1907(4)	-3396(2)	105.4(18)
O5S	-64(6)	4731(4)	-3404(3)	109.9(18)
O3S	2114(6)	5290(4)	4697(3)	103.0(16)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for (UO2)5(dpa)8(Gd)2(H2O)12;10H2O. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	20.74(7)	21.52(8)	21.36(8)	-3.73(6)	3.40(6)	-1.62(6)
U3	20.62(6)	33.01(7)	18.13(6)	-3.94(4)	4.65(4)	-9.00(5)

U2	21.99(6)	27.38(6)	20.57(6)	-4.25(4)	6.11(4)	-7.07(5)
Gd1	31.24(8)	24.30(8)	21.17(8)	-3.22(6)	8.39(6)	-4.87(6)
O81C	38.2(14)	57.9(18)	23.7(13)	-12.8(12)	11.2(10)	-25.8(13)
O6AA	39.3(14)	31.8(13)	31.8(14)	-10.5(10)	15.0(11)	-5.2(11)
N1C	23.9(13)	21.1(13)	21.1(13)	-3(1)	2.8(10)	-4.3(10)
O81A	49.3(15)	24.7(13)	36.1(14)	-3.5(10)	21.7(12)	-5.9(11)
O5W	37.5(14)	45.5(16)	34.9(15)	-6.8(12)	4.1(11)	-3.9(12)
N1A	25.9(13)	22.1(14)	30.1(15)	1.6(11)	4.8(11)	-0.6(11)
O71D	43.7(14)	32.9(13)	22.3(12)	-3.6(10)	11.2(10)	-12.0(11)
O4W	70(2)	30.7(14)	30.5(14)	-1.7(11)	18.2(13)	-4.6(14)
O2W	47.7(16)	45.7(17)	38.6(16)	-6.0(13)	-1.7(13)	-2.2(13)
N1D	27.4(14)	27.7(14)	20.1(13)	-0.3(11)	2.7(10)	-1.8(11)
O22Y	31.4(13)	31.6(13)	34.8(14)	2.0(11)	2.9(10)	-3.1(10)
O71C	32.1(13)	50.4(16)	27.7(13)	-14.6(11)	11.3(10)	-15.4(12)
O6W	79(2)	30.7(15)	45.3(18)	-10.6(12)	30.3(16)	-13.8(15)
O82C	35.4(13)	47.0(16)	24.1(12)	-6.5(11)	12.4(10)	-16.8(12)
N1B	24.9(13)	21.0(13)	22.4(13)	0.7(10)	7.7(10)	-4.1(10)
O11Y	27.5(13)	63(2)	38.8(16)	-7.8(14)	-8.3(11)	3.1(13)
O81D	56.4(17)	33.5(14)	32.8(14)	-0.3(11)	14.7(13)	-12.9(13)
O72B	57.1(17)	45.3(16)	34.2(15)	-19.3(12)	17.0(13)	-18.5(14)
O32Y	26.7(13)	54.6(18)	49.1(17)	-12.9(14)	-10.1(12)	-3.0(12)
O21Y	30.8(13)	35.8(15)	45.9(16)	1.4(12)	2.8(11)	-1.4(11)
O1W	47.1(15)	42.4(16)	37.6(15)	-15.8(12)	24.5(12)	-21.3(13)
O71B	41.8(15)	69(2)	42.4(16)	-31.0(15)	25.2(13)	-32.6(15)
O81B	45.1(15)	51.1(17)	27.0(13)	-8.7(12)	13.7(11)	-21.3(13)
C8C	30.7(17)	26.0(16)	22.4(16)	-0.9(12)	5.8(13)	-8.7(13)
O31Y	30.4(13)	67(2)	31.5(14)	9.5(13)	-4.7(11)	-11.6(13)
O3W	45.5(16)	40.5(17)	51.0(19)	5.2(13)	9.6(14)	7.9(13)
O19	62.3(19)	60(2)	40.0(17)	-6.2(14)	32.3(15)	-24.1(16)
O72D	39.1(14)	38.0(14)	25.0(12)	4.8(10)	2.6(10)	-13.9(11)
C2C	29.8(16)	22.9(16)	22.6(16)	-3.3(12)	1.6(12)	-3.6(13)
C6B	24.8(15)	22.6(16)	30.5(17)	4.0(13)	10.9(13)	-3.3(13)
O72C	48.7(16)	53.5(18)	26.8(13)	-19.6(12)	9.4(12)	-10.9(14)
C5C	27.3(16)	25.8(17)	31.6(18)	1.2(13)	3.5(13)	-7.4(13)
C6C	23.6(15)	23.8(16)	23.2(15)	-0.4(12)	2.8(12)	-3.9(12)
C7D	24.0(15)	33.2(18)	20.2(15)	2.7(13)	0.7(12)	-3.7(13)
C3C	36.8(19)	29.6(18)	29.6(18)	-3.2(14)	-3.3(15)	-8.2(15)
C7C	32.7(17)	29.4(18)	27.5(17)	-6.3(14)	4.6(14)	-2.9(14)
C6D	37.3(19)	27.4(18)	30.8(18)	-2.2(14)	4.5(15)	0.8(15)
C4C	28.2(17)	32.9(19)	39(2)	-1.2(15)	-5.0(15)	-10.5(15)
C2B	29.6(16)	24.5(16)	24.7(16)	0.3(12)	4.3(13)	-5.7(13)
C6A	19.0(14)	28.6(17)	27.3(17)	0.7(13)	0.9(12)	-2.9(12)
O82D	74(2)	29.4(15)	59(2)	-1.6(13)	8.9(17)	-12.0(15)
C5B	23.5(16)	31.2(19)	45(2)	6.8(15)	5.9(15)	-3.4(14)
C8A	23.8(15)	28.0(17)	28.2(17)	-4.5(13)	6.6(13)	-3.7(13)
C2A	41(2)	20.8(17)	46(2)	1.9(15)	15.8(17)	0.4(15)
C8D	42(2)	29.7(19)	37(2)	1.6(15)	1.5(16)	-3.6(16)
C3B	38.0(19)	31.7(19)	31.9(19)	2.2(14)	-6.7(15)	-10.5(16)

C4B	24.4(17)	37(2)	49(2)	9.3(17)	-4.7(16)	-7.8(15)
C5A	20.7(15)	44(2)	27.8(18)	5.2(15)	3.0(13)	-3.1(15)
C7B	36.2(18)	31.2(18)	28.2(18)	-5.8(14)	10.4(14)	-12.8(15)
C2D	27.6(16)	31.5(18)	19.0(15)	4.2(12)	0.7(12)	-0.7(14)
C4A	32.8(19)	42(2)	46(2)	20.7(18)	5.9(17)	-1.6(17)
C3D	50(2)	43(2)	20.0(17)	2.0(15)	8.9(15)	0.7(18)
C3A	49(2)	25.0(19)	66(3)	12.6(18)	17(2)	0.5(17)
C5D	75(3)	36(2)	35(2)	-10.1(17)	8(2)	-3(2)
C8B	36.2(19)	29.6(18)	33.0(19)	0.6(14)	15.0(15)	-8.9(15)
O71A	112(3)	26.5(15)	69(2)	-14.6(15)	61(2)	-19.7(17)
C4D	84(3)	47(3)	29(2)	-8.7(18)	17(2)	0(2)
C7A	94(4)	28(2)	75(4)	-12(2)	51(3)	-12(2)
O72A	202(5)	23.8(18)	144(4)	-23(2)	123(4)	-26(2)
O1S	66(2)	52(2)	51(2)	-2.8(15)	-10.9(16)	-11.5(16)
O2S	52.1(18)	45.1(18)	55(2)	-2.8(14)	7.5(15)	-1.8(14)
O4S	51(2)	178(5)	87(3)	-65(3)	1(2)	0(3)
O5S	86(3)	96(4)	156(5)	16(3)	-15(3)	-45(3)
O3S	141(4)	71(3)	96(4)	0(3)	26(3)	-14(3)

Table 4 Bond Lengths for (UO2)5(dpa)8(Gd)2(H2O)12;10H2O.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	O81A[1]	2.466(2)		O71C	C7C	1.283(4)
U1	O81A	2.466(2)		O82C	C8C	1.241(4)
U1	N1A	2.643(3)		N1B	C6B	1.329(4)
U1	N1A[1]	2.643(3)		N1B	C2B	1.341(4)
U1	O11Y	1.747(2)		O81D	C8D	1.272(5)
U1	O11Y[1]	1.747(2)		O72B	C7B	1.255(4)
U1	O71A[1]	2.486(3)		O71B	C7B	1.238(4)
U1	O71A	2.486(3)		O81B	C8B	1.243(4)
U3	O71D	2.369(2)		C8C	C6C	1.499(4)
U3	N1D	2.498(3)		O19	C8B[3]	1.251(4)
U3	O81D	2.380(3)		O72D	C7D	1.225(4)
U3	O72B	2.377(3)		C2C	C3C	1.384(5)
U3	O32Y	1.753(3)		C2C	C7C	1.509(5)
U3	O31Y	1.761(3)		C6B	C5B	1.382(5)
U3	O19	2.335(3)		C6B	C8B	1.495(5)
U2	O81C	2.459(2)		O72C	C7C	1.227(4)
U2	N1C	2.599(3)		C5C	C6C	1.384(4)
U2	O22Y	1.774(3)		C5C	C4C	1.382(5)
U2	O71C	2.405(2)		C7D	C2D	1.505(5)
U2	N1B	2.660(3)		C3C	C4C	1.385(5)
U2	O21Y	1.764(3)		C6D	C8D	1.506(5)
U2	O71B	2.504(3)		C6D	C5D	1.378(5)
U2	O81B	2.459(2)		C2B	C3B	1.386(5)
Gd1	O6AA	2.357(2)		C2B	C7B	1.483(5)
Gd1	O5W	2.411(3)		C6A	C8A	1.501(5)

Gd1	O4W	2.418(3)		C6A	C5A	1.380(5)
Gd1	O2W	2.418(3)		O82D	C8D	1.238(5)
Gd1	O6W	2.379(3)		C5B	C4B	1.378(6)
Gd1	O82C	2.408(2)		C8A	O6AA[2]	1.251(4)
Gd1	O1W	2.411(3)		C2A	C3A	1.388(6)
Gd1	O3W	2.424(3)		C2A	C7A	1.491(6)
O81C	C8C	1.264(4)		C3B	C4B	1.383(5)
O6AA	C8A[2]	1.251(4)		C5A	C4A	1.382(6)
N1C	C2C	1.341(4)		C2D	C3D	1.378(5)
N1C	C6C	1.334(4)		C4A	C3A	1.377(6)
O81A	C8A	1.255(4)		C3D	C4D	1.389(6)
N1A	C6A	1.332(4)		C5D	C4D	1.377(6)
N1A	C2A	1.334(4)		C8B	O19[3]	1.251(4)
O71D	C7D	1.284(4)		O71A	C7A	1.266(5)
N1D	C6D	1.339(4)		C7A	O72A	1.233(5)
N1D	C2D	1.334(4)				

[1]-X,-Y,1-Z; [2]1-X,-Y,-Z; [3]-X,-Y,-Z

II.29 U(dpa)$_2$(H$_2$O)$_2$·4(H$_2$O)

Table 1 Crystal data and structure refinement for U(dpa)2(H2O)2·4(H2O).	
Identification code	U(dpa)2(H2O)2·4(H2O)
Empirical formula	$C_{14}H_{10}N_2O_{14}U$
Formula weight	668.27
Temperature/K	299.65
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.8847(11)
b/Å	11.1134(9)
c/Å	12.8090(10)
α/°	90
β/°	103.042(4)
γ/°	90
Volume/Å^3	1925.5(3)
Z	4
ρ_{calc}g/cm^3	2.305
μ/mm^{-1}	8.509
F(000)	1248.0
Crystal size/mm^3	0.102 × 0.065 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.01 to 53.378
Index ranges	-17 ≤ h ≤ 17, -13 ≤ k ≤ 13, -15 ≤ l ≤ 15
Reflections collected	79853
Independent reflections	3930 [R_{int} = 0.0946, R_{sigma} = 0.0578]

Data/restraints/parameters	3930/0/257
Goodness-of-fit on F^2	1.125
Final R indexes [I>=2σ (I)]	R_1 = 0.0698, wR_2 = 0.1458
Final R indexes [all data]	R_1 = 0.0910, wR_2 = 0.1515
Largest diff. peak/hole / e $Å^{-3}$	2.97/-4.33

Table 2 Fractional Atomic Coordinates ($\times10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2\times10^3$) for U(dpa)2(H2O)2·4(H2O). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	2145.4(4)	2955.4(5)	3522.2(4)	24.60(17)
N1A	416(9)	2596(12)	3739(9)	28(3)
C2A	-198(11)	3559(15)	3753(12)	31(4)
C3A	-1168(15)	3390(20)	3782(15)	52(5)
C4A	-1524(12)	2250(20)	3755(15)	53(5)
C5A	-938(13)	1279(18)	3740(13)	44(4)
C6A	41(11)	1502(15)	3725(12)	29(4)
C7A	272(13)	4721(17)	3735(13)	38(4)
C8A	807(11)	559(14)	3710(11)	27(3)
O71A	1197(8)	4683(10)	3687(8)	32(2)
O72A	-167(10)	5680(11)	3798(10)	48(3)
O81A	1635(7)	931(9)	3679(8)	26(2)
O82A	594(9)	-555(11)	3724(10)	45(3)
N1B	3188(8)	4438(11)	4806(9)	25(3)
C2B	3632(12)	5363(15)	4418(14)	37(4)
C3B	4137(13)	6249(17)	5085(17)	48(5)
C4B	4170(15)	6213(18)	6171(16)	57(6)
C5B	3712(13)	-275(16)	1558(13)	42(4)
C6B	3247(10)	587(14)	882(11)	26(3)
C7B	3530(13)	5303(16)	3231(14)	39(4)
C8B	2682(10)	1630(13)	1196(11)	24(3)
O71B	3060(11)	4398(12)	2774(9)	51(4)
O72B	3916(10)	6084(12)	2792(11)	56(4)
O81B	2761(8)	1799(10)	2192(7)	32(3)
O82B	2199(7)	2742(9)	5461(7)	27(2)
O1W	1069(9)	3212(12)	1760(8)	47(3)
O2W	3732(9)	1962(13)	4296(9)	50(3)
O1S	5299(9)	724(12)	3969(10)	50(3)
O2S	1818(11)	7269(14)	3864(12)	69(4)
O3S	4519(12)	1749(15)	6388(13)	76(5)
O4S	3226(12)	-951(15)	4136(13)	74(4)

Table 3 Anisotropic Displacement Parameters ($Å^2\times10^3$) for U(dpa)2(H2O)2·4(H2O). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	25.2(3)	32.8(3)	16.4(3)	-1.5(3)	6.13(19)	-4.7(3)
N1A	27(7)	39(8)	15(6)	-3(5)	-1(5)	-4(6)

C2A	28(8)	41(10)	21(7)	-5(7)	-3(6)	-4(7)
C3A	53(12)	62(14)	39(10)	-9(9)	7(9)	13(10)
C4A	18(8)	87(17)	54(12)	-12(11)	8(8)	8(10)
C5A	37(10)	57(12)	34(9)	-7(9)	4(8)	-7(9)
C6A	23(8)	40(10)	23(8)	-2(7)	5(6)	-11(7)
C7A	35(10)	50(12)	27(8)	-4(8)	3(7)	0(8)
C8A	27(8)	34(9)	16(7)	-6(6)	-4(6)	-7(7)
O71A	31(6)	37(6)	29(6)	0(5)	9(5)	0(5)
O72A	57(8)	42(8)	44(7)	-5(6)	8(6)	16(6)
O82A	44(7)	41(8)	43(7)	4(6)	-7(6)	-8(6)
N1B	18(6)	35(7)	23(6)	1(5)	9(5)	-6(5)
C2B	31(9)	35(10)	46(10)	10(8)	8(8)	3(7)
C3B	32(9)	35(10)	72(14)	10(9)	-1(9)	-15(8)
C4B	56(12)	48(12)	50(12)	-6(10)	-21(10)	-24(10)
C5B	54(11)	37(10)	27(8)	1(7)	-9(8)	13(9)
C6B	17(7)	34(9)	25(7)	3(6)	-3(6)	1(6)
C7B	46(10)	33(10)	44(10)	-3(8)	22(9)	-5(8)
C8B	22(7)	28(8)	21(7)	3(6)	1(6)	-2(6)
O71B	89(10)	49(8)	22(6)	1(5)	30(7)	-12(7)
O72B	71(9)	42(8)	70(9)	2(7)	46(8)	-18(7)
O81B	39(6)	43(7)	15(5)	-4(4)	9(4)	1(5)
O82B	34(6)	36(6)	12(4)	3(4)	4(4)	-6(5)
O1W	59(8)	62(9)	16(5)	2(5)	-2(5)	37(7)
O2W	61(8)	55(8)	36(6)	-5(6)	10(6)	-14(7)

Table 4 Bond Lengths for U(dpa)2(H2O)2·4(H2O).

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	N1A	2.511(12)		C7A	O72A	1.24(2)
U1	O71A	2.364(11)		C8A	O81A	1.230(17)
U1	O81A	2.381(10)		C8A	O82A	1.275(19)
U1	N1B	2.538(12)		N1B	C2B	1.35(2)
U1	O71B	2.377(12)		N1B	$C6B^{1}$	1.362(18)
U1	O81B	2.438(9)		C2B	C3B	1.39(2)
U1	O82B	2.478(9)		C2B	C7B	1.50(2)
U1	O1W	2.426(10)		C3B	C4B	1.38(3)
U1	O2W	2.463(13)		C4B	$C5B^{1}$	1.37(3)
N1A	C2A	1.37(2)		C5B	$C4B^{2}$	1.37(3)
N1A	C6A	1.322(19)		C5B	C6B	1.35(2)
C2A	C3A	1.37(2)		C6B	$N1B^{2}$	1.362(18)
C2A	C7A	1.45(2)		C6B	C8B	1.50(2)
C3A	C4A	1.36(3)		C7B	O71B	1.27(2)
C4A	C5A	1.35(3)		C7B	O72B	1.22(2)
C5A	C6A	1.39(2)		C8B	O81B	1.269(16)
C6A	C8A	1.50(2)		C8B	$O82B^{2}$	1.240(16)
C7A	O71A	1.30(2)		O82B	$C8B^{1}$	1.240(16)

[1]+X,1/2-Y,1/2+Z; [2]+X,1/2-Y,-1/2+Z

II.30 Th(dpa)$_2$(H$_2$O)$_4$

Table 1 Crystal data and structure refinement for Th(dpa)2(H2O)4.	
Identification code	Th(dpa)2(H2O)4
Empirical formula	$C_{14}H_{14}N_2O_{12}Th$
Formula weight	634.31
Temperature/K	296.15
Crystal system	orthorhombic
Space group	Pbca
a/Å	6.4077(6)
b/Å	12.1860(11)
c/Å	43.280(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3379.5(5)
Z	8
ρ_{calc}g/cm^3	2.4932
μ/mm^{-1}	8.901
F(000)	2333.0
Crystal size/mm^3	0.209 × 0.107 × 0.098
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.76 to 60.94
Index ranges	-9 ≤ h ≤ 9, -14 ≤ k ≤ 17, -61 ≤ l ≤ 61
Reflections collected	88813
Independent reflections	5140 [R_{int} = 0.0833, R_{sigma} = 0.0410]
Data/restraints/parameters	5140/0/264
Goodness-of-fit on F^2	1.016
Final R indexes [I>=2σ (I)]	R_1 = 0.0305, wR_2 = 0.0790
Final R indexes [all data]	R_1 = 0.0545, wR_2 = 0.0999
Largest diff. peak/hole / e Å^{-3}	2.40/-2.67

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th(dpa)2(H2O)4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	5292.0(3)	3833.38(14)	1293.64(4)	15.06(7)
N2	4786(6)	3806(3)	1895.6(11)	17.7(9)
N1	5540(7)	3885(3)	689.7(10)	20.1(10)
O61b	6006(6)	5496(3)	1581.2(8)	22.8(8)
O4w	1699(5)	4489(3)	1486.7(8)	21.6(7)
O71b	4225(6)	2126(3)	1534.6(8)	23.7(8)
O71a	8417(5)	4671(3)	1055.6(8)	22.7(8)
O2w	8394(6)	3216(3)	1602.7(8)	28.8(9)

O3w	3843(6)	5598(3)	1029.1(8)	28.1(8)
O1w	7199(6)	2197(3)	1032.3(9)	32.7(9)
O61a	2477(6)	3065(3)	1002.8(8)	24.7(8)
O72a	10401(6)	5229(3)	660.0(9)	27.8(9)
O62b	6212(6)	6550(3)	2001.1(8)	27.6(8)
O72b	3726(6)	978(3)	1929.6(9)	27.0(9)
O62a	679(6)	2581(3)	583.8(9)	30.4(9)
C1b	5136(7)	4708(4)	2060.6(12)	17.5(10)
C3a	5896(11)	3811(4)	57.5(13)	29.7(12)
C3b	4392(9)	3750(4)	2528.6(13)	25.6(12)
C5a	7228(8)	4309(4)	550.4(11)	20.9(10)
C2b	4939(8)	4713(4)	2378.4(12)	21.5(11)
C5b	4283(8)	2863(4)	2039.6(11)	18.4(10)
C7b	4051(8)	1901(4)	1822.5(12)	19.3(10)
C6b	5833(8)	5673(4)	1873.0(11)	18(1)
C1a	4037(9)	3425(4)	519.7(12)	22.1(10)
C6a	2227(8)	2971(4)	709.1(12)	23.1(11)
C7a	8826(8)	4777(4)	767.2(11)	20.6(10)
C4b	4073(8)	2809(4)	2358.2(12)	23.7(11)
C2a	4138(9)	3381(5)	203.9(12)	27.1(12)
C4a	7444(9)	4286(4)	233.1(12)	29.0(12)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Th(dpa)2(H2O)4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Th1	16.03(12)	12.77(11)	16.38(11)	-1.16(6)	-0.25(6)	-0.05(6)
N2	19(2)	15(2)	19(2)	-2.7(15)	1.2(16)	3.4(15)
N1	21(2)	23(2)	16(2)	2.4(17)	-0.1(17)	1.9(16)
O61b	32(2)	16.6(18)	20.2(18)	-4.8(16)	-1.7(16)	-2.9(13)
O4w	18.0(18)	20.1(18)	26.6(19)	2.9(14)	0.9(15)	-0.6(14)
O71b	33(2)	14.1(17)	23.5(19)	-0.8(15)	1.9(16)	-0.2(14)
O71a	19.7(18)	29.2(19)	19.2(17)	-2.9(15)	-2.5(14)	-0.5(14)
O2w	20.6(19)	29(2)	37(2)	-3.3(16)	-4.5(16)	14.6(17)
O3w	34(2)	21(2)	29(2)	1.1(17)	-1.7(17)	1.3(15)
O1w	37(2)	19.4(19)	42(2)	6.4(17)	10.6(19)	-1.8(16)
O61a	23.2(19)	29(2)	21.4(19)	-7.3(16)	-1.7(15)	-2.2(15)
O72a	24(2)	33(2)	27(2)	-4.8(16)	2.1(16)	3.2(17)
O62b	40(2)	17.2(18)	25.5(19)	-7.6(18)	0.6(17)	-3.1(15)
O72b	35(2)	15.5(18)	30(2)	-6.4(16)	2.9(18)	4.2(14)
O62a	29(2)	34(2)	28(2)	-8.2(18)	-8.8(17)	-6.3(17)
C1b	20(2)	14(2)	19(2)	3.5(18)	-0.7(19)	-0.5(19)
C3a	36(3)	32(3)	21(3)	3(2)	4(3)	-1(2)
C3b	25(3)	34(3)	18(3)	5(2)	4(2)	-2(2)
C5a	19(3)	22(3)	22(3)	1(2)	5(2)	1(2)
C2b	23(3)	21(3)	21(3)	-2(2)	-2(2)	-1(2)
C5b	17(2)	18(2)	20(2)	2.0(19)	2.0(19)	2.2(18)

C7b	14(2)	16(2)	28(3)	-3.3(19)	1(2)	-1.0(19)
C6b	20(2)	14(2)	19(2)	2(2)	-1.1(19)	-1.4(18)
C1a	24(3)	20(3)	22(3)	2(2)	-5(2)	-1(2)
C6a	23(3)	20(2)	27(3)	0(2)	-7(2)	-1(2)
C7a	18(3)	22(3)	22(2)	4(2)	1(2)	1.7(19)
C4b	24(3)	22(3)	25(3)	1(2)	5(2)	5(2)
C2a	33(3)	28(3)	20(3)	1(3)	-6(2)	-4(2)
C4a	25(3)	35(3)	27(3)	4(3)	7(2)	6(2)

Table 4 Bond Lengths for Th(dpa)2(H2O)4.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	N2	2.625(5)		O61a	C6a	1.286(6)
Th1	N1	2.619(5)		O72a	C7a	1.239(6)
Th1	O61b	2.422(3)		O62b	C6b	1.229(6)
Th1	O4w	2.576(3)		O72b	C7b	1.234(6)
Th1	O71b	2.425(3)		O62a	C6a	1.227(6)
Th1	O71a	2.472(3)		C1b	C2b	1.381(7)
Th1	O2w	2.511(3)		C1b	C6b	1.497(7)
Th1	O3w	2.607(3)		C3a	C2a	1.395(9)
Th1	O1w	2.597(3)		C3a	C4a	1.377(8)
Th1	O61a	2.391(4)		C3b	C2b	1.387(7)
N2	C1b	1.330(6)		C3b	C4b	1.378(7)
N2	C5b	1.346(6)		C5a	C7a	1.501(7)
N1	C5a	1.342(6)		C5a	C4a	1.381(7)
N1	C1a	1.335(7)		C5b	C7b	1.510(7)
O61b	C6b	1.286(6)		C5b	C4b	1.387(7)
O71b	C7b	1.281(6)		C1a	C6a	1.524(8)
O71a	C7a	1.282(6)		C1a	C2a	1.370(7)

II.31 U-Mn-nic

Table 1 Crystal data and structure refinement for U-Mn-nic.

Identification code	U-Mn-nic
Empirical formula	$C_{73}H_{40}Cl_2Mn_2N_{12}O_{41.5}U_6$
Formula weight	3358.13
Temperature/K	299.18
Crystal system	monoclinic
Space group	C2/c
a/Å	38.333(5)
b/Å	17.355(2)
c/Å	18.670(2)
α/°	90
β/°	104.648(5)
γ/°	90

Volume/Å^3	12017(2)
Z	4
ρ_{calc}g/cm^3	1.856
μ/mm^{-1}	8.376
F(000)	6120.0
Crystal size/mm^3	0.176 × 0.117 × 0.067
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.59 to 46.61
Index ranges	-42 ≤ h ≤ 42, -19 ≤ k ≤ 19, -20 ≤ l ≤ 20
Reflections collected	122515
Independent reflections	8681 [R_{int} = 0.1217, R_{sigma} = 0.0631]
Data/restraints/parameters	8681/0/571
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0522, wR_2 = 0.1406
Final R indexes [all data]	R_1 = 0.0898, wR_2 = 0.1632
Largest diff. peak/hole / e Å^{-3}	2.50/-1.53

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Mn-nic. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	2721.4(2)	3880.0(3)	4540.0(3)	24.12(19)
U2	2834.1(2)	1729.0(3)	4074.4(3)	23.32(19)
U3	1905.1(2)	2571.2(3)	3933.4(3)	23.98(19)
Mn1	0	4249(4)	2500	70.6(15)
Mn2	5000	4474(4)	7500	109(2)
O72A	1883(3)	2006(7)	2736(6)	36(3)
O71B	2291(3)	4414(7)	3447(6)	37(3)
O71D	3559(3)	3419(7)	6201(7)	40(3)
O2	2842(4)	1413(9)	5293(6)	59(4)
O71A	2414(3)	1442(6)	2850(6)	32(3)
O72F	3052(3)	3805(7)	3626(7)	39(3)
O71E	1385(3)	3201(8)	4128(7)	43(3)
O72B	1799(3)	3673(7)	3125(6)	38(3)
O72D	3326(3)	4182(7)	5237(7)	44(3)
O71C	2238(4)	4664(7)	5959(7)	48(3)
O71F	3136(4)	2575(7)	3375(7)	48(4)
O72E	1540(3)	3671(9)	5286(7)	53(4)
O72C	2543(5)	4996(8)	5141(9)	82(6)
N1B	1805(4)	6011(8)	1840(7)	27(3)
N1A	2024(4)	346(8)	831(7)	33(3)
C7B	1967(5)	4307(9)	3110(9)	29(4)
C3A	1971(5)	1297(10)	1736(9)	35(4)
Cl	494(4)	4382(10)	1909(9)	92(4)
C2A	2108(5)	631(10)	1527(9)	36(5)
C6A	1798(6)	762(10)	341(10)	45(5)
C7A	2102(5)	1605(9)	2514(8)	28(4)
C2B	1959(5)	5437(9)	2276(9)	33(4)
C3B	1771(5)	4932(10)	2634(9)	36(4)

C7D	3576(5)	3952(10)	5734(11)	39(5)
C71F	3182(5)	3280(11)	3314(10)	38(5)
Cl1	5438(5)	4236(13)	6671(11)	114(6)
C6B	1458(6)	6129(11)	1773(10)	45(5)
C7E	1327(5)	3613(12)	4665(10)	40(5)
C5A	1651(7)	1444(13)	505(11)	71(8)
C5B	1244(6)	5664(13)	2101(12)	59(6)
C3E	974(5)	3989(14)	4501(11)	55(6)
N1C	2468(6)	6810(12)	7018(13)	80(6)
C7C	2390(11)	5111(12)	5650(20)	136(17)
C31F	3407(7)	3554(13)	2810(13)	66(7)
C4B	1410(5)	5041(12)	2522(11)	49(5)
C4A	1727(6)	1711(13)	1207(11)	64(7)
C3C	2487(7)	5954(13)	6038(14)	65(7)
C2E	723(5)	3946(13)	3846(12)	56(6)
C3D	3940(6)	4292(13)	5768(11)	54(6)
C5C	2671(9)	7215(17)	5941(16)	97(10)
C4C	2625(8)	6528(12)	5644(17)	88(9)
C6C	2595(8)	7357(18)	6629(17)	92(9)
C2C	2421(8)	6168(15)	6707(14)	81(8)
C2D	4223(6)	4209(15)	6390(13)	66(7)
N1E	397(5)	4289(15)	3682(11)	87(7)
N1D	4548(5)	4517(15)	6438(13)	93(8)
C4D	3992(7)	4673(17)	5182(15)	95(10)
O3B	2229(6)	1380(20)	4157(15)	44(8)
C6E	318(7)	4720(20)	4219(16)	138(18)
C4E	877(7)	4447(19)	5052(14)	97(11)
C5E	548(8)	4800(20)	4893(16)	129(15)
C5D	4336(7)	5030(20)	5220(20)	151(19)
O73	5000	5850(30)	7500	173(16)
C6D	4607(8)	4940(20)	5870(20)	130(15)
O3A	2287(7)	1740(20)	4366(15)	10(11)
O4B	2467(6)	2883(13)	3584(18)	23(9)
C1G	-90(20)	2470(20)	2650(50)	150(30)
O11G	89(11)	2972(19)	2440(30)	91(12)
O12G	-126(13)	1770(20)	2550(30)	150(20)
O2W	0	5620(60)	2500	220(40)
C42F	3511(10)	4280(20)	2770(20)	119(11)
C52F	3688(10)	4540(20)	2230(20)	122(12)
C62F	3855(12)	3960(30)	1920(30)	158(16)
N12F	3724(8)	3222(19)	1862(17)	128(10)
C21F	3524(7)	3011(16)	2361(15)	78(7)
O4A	2479(5)	2730(12)	3985(16)	21(8)
O0AA	3066(6)	2737(8)	4851(7)	84(6)
O2AA	1521(17)	6090(40)	4830(40)	180(20)
O1AA	1690(9)	5055(19)	4391(19)	77(10)
O1	434(7)	4891(16)	2112(15)	50(7)
O33	5435(15)	4720(40)	6840(30)	150(20)

O3AA	3848(11)	2850(20)	4620(20)	238(17)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Mn-nic. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
U1	36.3(4)	18.2(3)	16.8(3)	-0.6(3)	4.8(3)	-2.3(3)
U2	33.6(4)	20.9(3)	14.7(3)	-2.4(2)	4.5(3)	0.1(3)
U3	34.6(4)	20.6(3)	15.3(3)	-1.6(3)	3.7(3)	-1.6(3)
Mn1	47(3)	97(4)	59(3)	0	-4(2)	0
Mn2	61(4)	102(5)	135(6)	0	-28(4)	0
O72A	44(8)	42(7)	21(6)	-10(6)	5(6)	6(6)
O71B	43(8)	33(7)	27(7)	12(6)	-3(6)	1(6)
O71D	42(8)	34(7)	34(7)	-3(6)	-7(6)	-16(6)
O2	69(10)	88(11)	20(7)	-15(7)	8(6)	-62(9)
O71A	48(8)	31(7)	12(6)	-6(5)	-2(6)	0(6)
O72F	59(8)	29(7)	33(7)	-3(6)	20(6)	-9(6)
O71E	28(7)	60(9)	34(7)	-3(7)	-2(6)	15(6)
O72B	44(8)	33(7)	29(7)	10(6)	-4(6)	-6(6)
O72D	38(8)	31(7)	51(8)	17(6)	-11(7)	-7(6)
O71C	76(10)	28(7)	54(8)	-5(6)	41(8)	3(7)
O71F	77(10)	28(8)	54(9)	6(6)	43(8)	6(7)
O72E	30(7)	88(11)	37(8)	-30(8)	2(6)	8(7)
O72C	165(17)	33(8)	86(12)	-22(8)	102(13)	-25(9)
N1A	43(9)	26(8)	27(8)	-4(7)	1(7)	10(7)
C7B	47(12)	21(10)	17(9)	4(7)	5(9)	2(9)
C3A	50(12)	29(10)	24(9)	-12(8)	4(9)	0(9)
C2A	60(13)	33(11)	14(9)	2(8)	10(8)	7(9)
C6A	72(15)	32(11)	23(10)	-14(9)	-2(10)	6(10)
C7A	50(12)	16(9)	11(8)	0(7)	-2(9)	4(9)
C2B	48(11)	19(9)	33(10)	12(8)	14(9)	-13(8)
C3B	42(12)	37(11)	28(10)	5(8)	8(9)	-5(9)
C7D	50(13)	19(10)	44(12)	-2(9)	9(10)	2(9)
C71F	41(11)	39(12)	32(10)	-4(9)	8(9)	6(10)
C6B	67(14)	34(11)	36(11)	13(9)	17(10)	5(10)
C7E	34(11)	62(13)	27(11)	-13(10)	11(9)	6(10)
C5A	110(20)	61(15)	27(12)	-4(11)	-10(12)	33(15)
C5B	50(14)	60(15)	68(15)	16(13)	17(12)	4(12)
C3E	38(12)	81(16)	39(12)	2(11)	-4(10)	16(12)
N1C	93(17)	50(13)	102(18)	-7(13)	36(14)	-10(12)
C7C	260(40)	15(12)	220(40)	9(17)	220(40)	10(17)
C31F	100(20)	46(13)	65(15)	13(12)	49(15)	-18(13)
C4B	42(13)	62(14)	47(12)	14(11)	22(10)	-3(11)
C4A	82(17)	59(14)	34(12)	-7(11)	-19(11)	39(13)
C3C	84(18)	57(15)	72(16)	6(13)	50(14)	21(13)
C2E	35(12)	77(16)	50(13)	-15(12)	-1(10)	27(12)
C3D	50(14)	65(15)	42(12)	6(11)	3(11)	-12(11)

C5C	140(30)	70(20)	90(20)	15(17)	50(20)	-25(19)
C4C	150(30)	18(12)	110(20)	0(13)	70(20)	3(14)
C6C	100(20)	90(20)	100(20)	-47(19)	33(18)	-21(18)
C2C	120(20)	53(17)	71(18)	5(14)	35(17)	10(16)
C2D	39(13)	96(19)	59(15)	11(14)	3(11)	-8(13)
N1E	60(14)	130(20)	65(14)	-17(14)	-5(11)	21(14)
N1D	41(12)	130(20)	105(18)	35(16)	3(12)	-25(13)
C4D	71(18)	120(20)	78(19)	62(18)	-18(15)	-7(17)
C6E	69(19)	240(40)	80(20)	-70(30)	-30(16)	100(20)
C4E	59(17)	160(30)	58(16)	-36(18)	-3(13)	58(19)
C5E	80(20)	230(40)	70(19)	-60(20)	12(16)	60(20)
C5D	49(18)	210(40)	180(40)	130(30)	10(20)	-30(20)
C6D	59(19)	180(40)	140(30)	90(30)	10(20)	-30(20)
O0AA	190(19)	28(8)	16(7)	1(6)	-8(9)	-6(10)

Table 4 Bond Lengths for U-Mn-nic.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	U3	3.8004(9)		O72B	C7B	1.28(2)
U1	O71B	2.458(11)		O72D	C7D	1.22(2)
U1	O2^{1}	2.316(13)		O71C	U2^{1}	2.433(12)
U1	O72F	2.372(12)		O71C	C7C	1.20(2)
U1	O72D	2.412(12)		O71F	C71F	1.25(2)
U1	O72C	2.423(13)		O72E	U2^{1}	2.493(12)
U1	N1A^{2}	2.872(13)		O72E	C7E	1.24(2)
U1	O3B^{1}	2.43(2)		O72C	C7C	1.26(3)
U1	O3A^{1}	2.31(2)		N1B	U2^{2}	2.753(13)
U1	O4B	2.50(2)		N1B	C2B	1.33(2)
U1	O4A	2.331(19)		N1B	C6B	1.32(2)
U1	O0AA	2.373(16)		N1A	U1^{3}	2.872(13)
U2	U3	3.7964(10)		N1A	C2A	1.35(2)
U2	O2	2.333(12)		N1A	C6A	1.31(2)
U2	O71A	2.490(11)		C7B	C3B	1.48(2)
U2	O71C^{1}	2.433(12)		C3A	C2A	1.36(2)
U2	O71F	2.444(12)		C3A	C7A	1.51(2)
U2	O72E^{1}	2.493(12)		C3A	C4A	1.38(3)
U2	N1B^{3}	2.753(13)		C6A	C5A	1.38(3)
U2	O3B	2.44(2)		C2B	C3B	1.41(2)
U2	O3A	2.30(2)		C3B	C4B	1.36(3)
U2	O4B	2.49(3)		C7D	C3D	1.50(3)
U2	O4A	2.19(2)		C71F	C31F	1.51(3)
U2	O0AA	2.302(13)		Cl1	O33	0.90(6)
U3	U2^{1}	3.7986(9)		C6B	C5B	1.40(3)
U3	O72A	2.422(11)		C7E	C3E	1.46(3)
U3	O71D^{1}	2.441(11)		C5A	C4A	1.35(3)
U3	O2^{1}	2.329(12)		C5B	C4B	1.39(3)
U3	O71E	2.381(12)		C3E	C2E	1.35(3)

U3	O72B	2.406(11)		C3E	C4E	1.42(3)
U3	O3B	2.39(3)		N1C	C6C	1.36(3)
U3	O3A	2.07(2)		N1C	C2C	1.25(3)
U3	O4B	2.46(3)		C7C	C3C	1.63(4)
U3	O4A	2.20(2)		C31F	C42F	1.33(4)
U3	O0AA[1]	2.308(13)		C31F	C21F	1.41(3)
Mn1	Cl[4]	2.433(15)		C3C	C4C	1.42(3)
Mn1	Cl	2.433(16)		C3C	C2C	1.39(3)
Mn1	N1E	2.343(19)		C2E	N1E	1.35(3)
Mn1	N1E[4]	2.343(19)		C3D	C2D	1.38(3)
Mn1	O11G	2.25(3)		C3D	C4D	1.34(3)
Mn1	O2W	2.38(11)		C5C	C4C	1.31(3)
Mn1	O1	2.27(3)		C5C	C6C	1.41(4)
Mn1	O1[4]	2.27(3)		C2D	N1D	1.34(3)
Mn2	Cl1[5]	2.59(2)		N1E	C6E	1.34(3)
Mn2	Cl1	2.59(2)		N1D	C6D	1.35(3)
Mn2	N1D[5]	2.28(2)		C4D	C5D	1.44(4)
Mn2	N1D	2.28(2)		O3B	U1[1]	2.43(2)
Mn2	O73	2.39(4)		C6E	C5E	1.35(3)
Mn2	O33[5]	2.35(6)		C4E	C5E	1.36(3)
Mn2	O33	2.35(6)		C5D	C6D	1.39(4)
O72A	C7A	1.24(2)		O3A	U1[1]	2.31(2)
O71B	C7B	1.26(2)		C1G	O11G	1.2374
O71D	U3[1]	2.441(11)		C1G	O12G	1.2367
O71D	C7D	1.28(2)		C42F	C52F	1.42(5)
O2	U1[1]	2.316(13)		C52F	C62F	1.38(5)
O2	U3[1]	2.329(12)		C62F	N12F	1.37(5)
O71A	C7A	1.24(2)		N12F	C21F	1.40(4)
O72F	C71F	1.25(2)		O0AA	U3[1]	2.308(13)
O71E	C7E	1.30(2)				

[1]1/2-X,1/2-Y,1-Z; [2]1/2-X,1/2+Y,1/2-Z; [3]1/2-X,-1/2+Y,1/2-Z; [4]-X,+Y,1/2-Z; [5]1-X,+Y,3/2-Z

Table 5 Atomic Occupancy for U-Mn-nic.

Atom	***Occupancy***		**Atom**	***Occupancy***		**Atom**	***Occupancy***
Cl	0.5		Cl1	0.5		O3B	0.61(6)
O3A	0.39(6)		O4B	0.48(5)		C1G	0.5
O11G	0.5		O12G	0.5		O2W	0.5
O4A	0.52(5)		O2AA	0.5		O1AA	0.5
O1	0.5		O33	0.5			

II.32 U-Fe-nic

Table 1 Crystal data and structure refinement for U-Fe-nic.	
Identification code	U-Fe-nic
Empirical formula	$C_{73}H_{53}Cl_2Fe_2N_{12}O_{39.5}U_6$

Formula weight	3341.05
Temperature/K	100
Crystal system	monoclinic
Space group	C2/c
a/Å	37.963(5)
b/Å	17.283(2)
c/Å	18.561(2)
α/°	90
β/°	104.911(4)
γ/°	90
Volume/Å^3	11768(3)
Z	4
ρ_{calc}g/cm^3	1.886
μ/mm^{-1}	7.332
F(000)	6116.0
Crystal size/mm^3	0.1 × 0.051 × 0.051
Radiation	AgKα (λ = 0.56086)
2Θ range for data collection/°	2.574 to 41.482
Index ranges	-47 ≤ h ≤ 47, -21 ≤ k ≤ 21, -23 ≤ l ≤ 23
Reflections collected	189142
Independent reflections	12191 [R_{int} = 0.1421, R_{sigma} = 0.0554]
Data/restraints/parameters	12191/0/571
Goodness-of-fit on F^2	1.100
Final R indexes [I>=2σ (I)]	R_1 = 0.0496, wR_2 = 0.1369
Final R indexes [all data]	R_1 = 0.0926, wR_2 = 0.2074
Largest diff. peak/hole / e Å^{-3}	3.60/-4.08

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U-Fe-nic. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	7163.5(2)	3261.6(3)	5931.7(2)	15.64(14)
U2	7276.6(2)	1111.6(3)	5453.4(2)	16.36(15)
U3	6895.2(2)	2580.0(3)	3922.0(2)	15.92(14)
Fe2	5000	4282(4)	2500	68.6(16)
O71B	7287(3)	4435(6)	3461(6)	25(2)
O71A	7411(3)	1438(6)	2835(5)	24(2)
O72B	6780(3)	3700(6)	3124(6)	27(2)
O72A	6870(3)	2023(6)	2719(6)	24(2)
O71E	6422(3)	1574(6)	3769(6)	26(2)
O72D	6942(3)	1161(6)	6380(6)	23(2)
O72E	6658(4)	795(7)	4730(7)	36(3)
O72F	6522(3)	3673(9)	5285(7)	44(4)
N1A	7014(4)	344(8)	809(7)	23(3)
O71F	6355(3)	3206(7)	4120(6)	29(3)
N1B	6801(3)	6039(7)	1859(7)	20(3)
O71D	6856(4)	2397(7)	6633(7)	36(3)
C7B	6958(4)	4330(9)	3108(8)	22(3)
C2A	7114(5)	640(9)	1506(9)	26(4)

C3B	6761(5)	4982(9)	2655(9)	25(3)
C7A	7097(4)	1629(9)	2485(8)	23(3)
C3A	6970(4)	1306(9)	1714(8)	21(3)
C2B	6955(5)	5456(9)	2298(9)	27(4)
C2C	7414(6)	6121(12)	6728(13)	45(5)
C6A	6775(6)	764(10)	284(9)	36(4)
N1C	7481(5)	6840(12)	7038(11)	53(5)
C7D	6818(5)	1678(10)	6694(9)	31(4)
C5A	6622(6)	1437(13)	445(9)	49(6)
C7F	6303(4)	3610(11)	4669(9)	30(4)
C3C	7472(7)	5921(12)	6035(11)	47(5)
C7E	6406(5)	1032(10)	4232(10)	33(4)
C4B	6392(5)	5082(10)	2567(10)	31(4)
C4A	6714(6)	1727(11)	1174(11)	44(5)
C7C	7425(7)	5132(12)	5721(13)	50(6)
C5C	7682(8)	7275(13)	5974(14)	60(6)
C6C	7606(7)	7411(14)	6662(14)	58(6)
C3D	6591(6)	1435(12)	7225(12)	46(5)
C4C	7620(7)	6535(12)	5667(12)	56(7)
C5B	6226(5)	5734(12)	2139(11)	40(5)
C6B	6443(5)	6178(11)	1794(10)	32(4)
C3F	5955(5)	3993(15)	4519(11)	50(6)
C2D	6471(8)	1988(15)	7669(15)	63(7)
C3E	6051(6)	703(13)	4212(12)	47(5)
C2F	5714(5)	3970(15)	3826(12)	53(6)
C4F	5856(7)	4430(20)	5063(14)	85(11)
C4E	5996(7)	254(15)	4813(15)	63(7)
O4B	6849(8)	2256(12)	5173(11)	30(7)
C2E	5766(7)	808(16)	3575(16)	68(7)
O71C	7235(4)	4680(7)	5977(7)	36(3)
O72C	7537(5)	5006(7)	5154(9)	64(6)
N1F	5384(7)	4357(16)	3659(15)	85(7)
C5F	5505(8)	4810(30)	4911(16)	115(16)
N1E	5432(6)	470(20)	3496(19)	109(11)
Fe1	5000	532(6)	2500	137(4)
C4D	6530(11)	680(20)	7270(20)	109(12)
C5D	6326(10)	360(20)	7800(20)	103(11)
O2	7147(4)	3596(10)	4709(6)	57(5)
O3B	7222(6)	1324(15)	4137(13)	21(7)
C6F	5306(10)	4810(30)	4242(18)	170(30)
Cl1	5477(9)	673(19)	1700(18)	168(11)
O4A	7029(7)	2254(11)	5122(10)	-1(7)
O3A	7287(5)	1690(14)	4359(12)	15(7)
O1	7528(4)	2159(9)	6233(14)	94(8)
N1D	6277(8)	1773(15)	8141(15)	96(10)
C6D	6226(10)	950(20)	8210(20)	102(11)
C5E	5647(10)	-60(30)	4780(30)	150(20)
C2	4916(13)	2530(20)	2570(40)	75(17)

O2AA	5124(11)	3020(20)	2420(20)	23(9)
O5	4894(13)	1820(20)	2510(40)	49(15)
O20	5000	-760(50)	2500	130(30)
O1AA	6669(9)	5240(30)	4640(30)	250(30)
O0AA	6142(9)	2166(19)	5440(18)	136(10)
Cl2	5494(4)	4529(9)	1979(9)	78(4)
C6E	5336(18)	-30(40)	4160(40)	180(20)
O3AA	5380(8)	5254(18)	2185(18)	131(10)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for U-Fe-nic. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	22.6(3)	16.8(3)	7.8(2)	-1.72(17)	4.52(18)	-0.32(18)
U2	25.4(3)	14.5(3)	10.0(2)	-0.67(16)	5.97(19)	-2.34(18)
U3	24.0(3)	15.6(3)	8.5(2)	-1.19(17)	4.71(18)	-1.41(18)
Fe2	28(2)	127(5)	41(3)	0	-8.8(19)	0
O71B	32(6)	24(6)	19(5)	14(4)	6(5)	1(5)
O71A	44(7)	15(5)	10(5)	-2(4)	2(5)	7(5)
O72B	39(7)	19(6)	25(6)	5(4)	11(5)	-11(5)
O72A	30(6)	26(6)	14(5)	-10(4)	1(4)	13(5)
O71E	24(6)	25(6)	26(6)	6(5)	0(5)	0(5)
O72D	30(6)	23(6)	19(5)	-1(4)	10(4)	-1(5)
O72E	44(8)	22(6)	36(7)	13(5)	-3(6)	-4(5)
O72F	29(7)	82(11)	19(6)	-20(6)	-1(5)	9(7)
N1A	29(7)	25(7)	11(6)	-9(5)	0(5)	0(6)
O71F	34(6)	42(7)	9(5)	-9(5)	6(4)	-2(5)
N1B	15(6)	23(7)	22(6)	12(5)	6(5)	-3(5)
O71D	60(9)	19(6)	43(7)	10(5)	38(7)	10(6)
C7B	31(9)	25(8)	11(7)	2(6)	5(6)	0(6)
C2A	38(9)	20(8)	19(8)	0(6)	3(7)	7(7)
C3B	38(9)	21(8)	19(7)	10(6)	10(7)	-8(7)
C7A	31(9)	24(8)	9(7)	-6(6)	-2(6)	12(6)
C3A	37(9)	20(8)	7(6)	-3(5)	7(6)	3(6)
C2B	37(9)	22(8)	23(8)	1(6)	6(7)	-2(7)
C2C	44(12)	37(11)	59(13)	1(9)	22(10)	-17(9)
C6A	64(13)	27(9)	14(8)	-5(6)	4(8)	15(8)
N1C	47(11)	68(13)	48(11)	4(9)	21(9)	11(9)
C7D	52(11)	23(9)	18(8)	9(6)	11(7)	0(8)
C5A	71(15)	52(13)	13(8)	2(8)	-10(8)	41(11)
C7F	20(8)	48(11)	21(8)	1(7)	4(6)	11(7)
C3C	78(16)	34(11)	36(11)	6(8)	28(10)	3(10)
C7E	34(10)	22(9)	38(10)	5(7)	2(8)	-4(7)
C4B	28(9)	27(9)	40(10)	8(7)	13(7)	2(7)
C4A	55(13)	32(10)	34(10)	-9(8)	-6(9)	25(9)
C7C	76(16)	29(11)	55(13)	-11(9)	36(12)	-13(10)
C5C	84(18)	30(12)	68(16)	7(11)	23(14)	4(11)

C6C	74(17)	53(14)	54(14)	-22(11)	28(13)	-7(12)
C3D	71(15)	34(11)	41(11)	-3(9)	30(11)	2(10)
C4C	100(20)	35(11)	44(12)	19(9)	43(13)	24(12)
C5B	27(9)	49(12)	45(11)	19(9)	10(8)	2(8)
C6B	32(9)	42(11)	24(9)	7(7)	9(7)	4(8)
C3F	27(10)	91(18)	29(10)	-23(10)	2(8)	9(10)
C2D	83(18)	51(14)	75(17)	-5(12)	55(15)	-3(13)
C3E	41(12)	50(13)	45(12)	14(10)	0(9)	-6(9)
C2F	32(11)	83(17)	39(11)	-8(11)	-1(9)	32(11)
C4F	52(15)	160(30)	37(13)	-35(16)	7(11)	30(17)
C4E	50(14)	66(17)	73(17)	28(13)	17(12)	-5(12)
C2E	47(14)	74(18)	70(17)	8(14)	-8(12)	-17(13)
O71C	56(8)	25(6)	39(7)	-3(5)	33(6)	-4(6)
O72C	133(15)	19(7)	80(11)	-15(7)	100(12)	-28(8)
C5F	80(20)	210(40)	45(15)	-50(20)	-10(14)	80(20)
N1E	42(13)	140(30)	130(30)	30(20)	-5(15)	-2(15)
Fe1	55(4)	142(8)	177(9)	0	-35(5)	0
O2	59(9)	105(13)	8(5)	-15(7)	8(6)	-66(9)
C6F	120(30)	320(70)	60(20)	-40(30)	-10(20)	170(40)
O1	18(7)	46(10)	210(20)	-87(13)	15(10)	-5(6)
N1D	150(30)	74(17)	100(20)	-18(14)	100(20)	-7(16)
C5E	70(20)	180(50)	180(50)	120(40)	0(30)	-20(30)
O1AA	100(20)	240(50)	370(70)	210(50)	10(30)	10(30)

Table 4 Bond Lengths for U-Fe-nic.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	U3	3.7927(8)		N1B	C2B	1.33(2)
U1	O71A^{1}	2.492(10)		N1B	C6B	1.35(2)
U1	O72F	2.525(12)		O71D	C7D	1.26(2)
U1	N1B^{2}	2.744(12)		C7B	C3B	1.49(2)
U1	O71D	2.463(11)		C2A	C3A	1.37(2)
U1	O4B	2.36(2)		C3B	C2B	1.38(2)
U1	O71C	2.465(12)		C3B	C4B	1.38(2)
U1	O2	2.327(12)		C7A	C3A	1.496(19)
U1	O3B^{1}	2.48(2)		C3A	C4A	1.41(2)
U1	O4A	2.271(19)		C2C	N1C	1.37(3)
U1	O3A^{1}	2.29(2)		C2C	C3C	1.40(3)
U1	O1	2.337(17)		C6A	C5A	1.37(3)
U2	U3^{1}	3.8036(8)		N1C	C6C	1.36(3)
U2	O71B^{1}	2.446(10)		C7D	C3D	1.52(3)
U2	O72D	2.387(11)		C5A	C4A	1.40(3)
U2	O72E	2.449(12)		C7F	C3F	1.44(3)
U2	N1A^{3}	2.846(13)		C3C	C7C	1.47(3)
U2	O4B	2.53(2)		C3C	C4C	1.45(3)
U2	O72C^{1}	2.432(13)		C7E	C3E	1.45(3)
U2	O2^{1}	2.339(13)		C4B	C5B	1.43(2)

U2	O3B	2.43(2)		C7C	O71C	1.24(2)
U2	O4A	2.205(19)		C7C	O72C	1.25(2)
U2	O3A	2.27(2)		C5C	C6C	1.40(3)
U2	O1	2.360(14)		C5C	C4C	1.40(3)
U3	U1[1]	3.8027(8)		C3D	C2D	1.41(3)
U3	O72B	2.408(11)		C3D	C4D	1.32(4)
U3	O72A	2.410(10)		C5B	C6B	1.40(3)
U3	O71E	2.464(11)		C3F	C2F	1.37(3)
U3	O71F	2.428(12)		C3F	C4F	1.39(3)
U3	O4B	2.44(2)		C2D	N1D	1.33(3)
U3	O2	2.328(13)		C3E	C4E	1.42(3)
U3	O3B	2.48(2)		C3E	C2E	1.39(3)
U3	O4A	2.225(18)		C2F	N1F	1.38(3)
U3	O3A	2.15(2)		C4F	C5F	1.45(4)
U3	O1[1]	2.327(16)		C4E	C5E	1.42(4)
Fe2	N1F	2.27(3)		C2E	N1E	1.36(3)
Fe2	N1F[4]	2.27(3)		O72C	U2[1]	2.432(13)
Fe2	O2AA	2.25(4)		N1F	C6F	1.43(4)
Fe2	Cl2[4]	2.359(16)		C5F	C6F	1.28(4)
Fe2	Cl2	2.359(16)		N1E	Fe1	2.14(3)
Fe2	O3AA[4]	2.38(3)		N1E	C6E	1.62(7)
Fe2	O3AA	2.38(3)		Fe1	N1E[4]	2.14(3)
O71B	U2[1]	2.446(10)		Fe1	Cl1	2.63(3)
O71B	C7B	1.264(19)		Fe1	Cl1[4]	2.63(3)
O71A	U1[1]	2.492(10)		Fe1	O5	2.26(4)
O71A	C7A	1.246(19)		Fe1	O20	2.24(9)
O72B	C7B	1.286(19)		C4D	C5D	1.51(5)
O72A	C7A	1.261(18)		C5D	C6D	1.38(5)
O71E	C7E	1.28(2)		O2	U2[1]	2.339(13)
O72D	C7D	1.23(2)		O3B	U1[1]	2.48(2)
O72E	C7E	1.22(2)		O3A	U1[1]	2.29(2)
O72F	C7F	1.23(2)		O1	U3[1]	2.327(16)
N1A	U2[5]	2.846(13)		N1D	C6D	1.45(4)
N1A	C2A	1.352(19)		C5E	C6E	1.42(7)
N1A	C6A	1.36(2)		C2	O2AA	1.2372
O71F	C7F	1.29(2)		C2	O5	1.2374
N1B	U1[6]	2.744(12)		Cl2	O3AA	1.41(3)

[1]3/2-X,1/2-Y,1-Z; [2]+X,1-Y,1/2+Z; [3]+X,-Y,1/2+Z; [4]1-X,+Y,1/2-Z; [5]+X,-Y,-1/2+Z; [6]+X,1-Y,-1/2+Z

II.33 $Np_2(1,4\text{-bdc})_4(DMF)_4$

Table 1 Crystal data and structure refinement for Np2(1,4-bdc)4(DMF)4.	
Identification code	Np2(1,4-bdc)4(DMF)4
Empirical formula	$C_{22}H_{22}N_2NpO_{10}$
Formula weight	711.41
Temperature/K	297.31

Crystal system	monoclinic
Space group	C2/c
a/Å	15.3450(7)
b/Å	11.4621(4)
c/Å	13.3406(6)
α/°	90
β/°	101.4300(10)
γ/°	90
Volume/Å^3	2299.89(17)
Z	4
ρ_{calc}g/cm^3	2.055
μ/mm^{-1}	4.580
F(000)	1364.0
Crystal size/mm^3	0.037 × 0.02 × 0.017
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.746 to 50.05
Index ranges	-18 ≤ h ≤ 18, -13 ≤ k ≤ 13, -15 ≤ l ≤ 15
Reflections collected	13623
Independent reflections	2029 [R_{int} = 0.0667, R_{sigma} = 0.0481]
Data/restraints/parameters	2029/3/164
Goodness-of-fit on F^2	1.130
Final R indexes [I>=2σ (I)]	R_1 = 0.0329, wR_2 = 0.0507
Final R indexes [all data]	R_1 = 0.0435, wR_2 = 0.0525
Largest diff. peak/hole / e Å^{-3}	1.11/-1.79

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np2(1,4-bdc)4(DMF)4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Np1	5000	1302.8(2)	7500	18.37(12)
O1	5266(3)	3228(3)	8324(3)	36.9(10)
O2	5458(3)	9343(3)	6979(3)	40.2(10)
O3	6423(3)	1992(4)	7176(3)	45.5(11)
O4	5529(3)	1372(3)	5842(3)	40.4(10)
O5	3827(3)	817(3)	6165(3)	39.3(10)
N1	2769(3)	821(4)	4740(4)	39.4(13)
C1	5000	3782(7)	7500	30.1(18)
C2	5000	5095(7)	7500	32(2)
C3	4828(4)	5678(5)	8328(5)	38.7(16)
C4	4795(4)	6883(5)	8327(5)	43.3(16)
C5	5000	7508(6)	7500	33(2)
C6	5000	8842(6)	7500	21.8(15)
C7	6229(3)	1820(4)	6258(4)	16.3(11)
C8	6902(4)	2164(5)	5609(5)	33.5(14)
C9	6711(4)	1969(5)	4562(5)	41.8(16)
C10	7301(4)	2293(5)	3957(5)	42.7(16)
C11	3598(4)	839(4)	5227(5)	34.9(15)
C12	2053(4)	773(7)	5299(6)	65(2)
C13	2520(5)	792(7)	3623(5)	67(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Np2(1,4-bdc)4(DMF)4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	21.09(18)	11.90(15)	23.98(19)	0	8.93(12)	0
O1	51(3)	18.9(19)	40(3)	-2.8(18)	7(2)	-0.2(18)
O2	51(3)	20(2)	55(3)	-4.1(19)	25(2)	0.7(19)
O3	32(2)	59(3)	49(3)	6(2)	15(2)	-11(2)
O4	40(2)	40(2)	45(2)	2(2)	19(2)	-7(2)
O5	37(2)	45(2)	34(3)	-8.0(19)	1(2)	-7.3(19)
N1	29(3)	47(3)	40(3)	0(2)	1(3)	2(2)
C1	33(4)	14(4)	45(5)	0	12(4)	0
C2	27(5)	30(4)	41(6)	0	12(4)	0
C3	58(4)	20(3)	43(4)	6(3)	22(3)	-5(3)
C4	56(4)	26(3)	53(4)	2(3)	21(4)	-7(3)
C5	39(5)	15(3)	43(5)	0	6(4)	0
C6	22(4)	22(3)	23(4)	0	9(3)	0
C7	18(3)	17(2)	16(3)	-1(2)	7(2)	-6(2)
C8	33(4)	35(3)	33(4)	0(3)	6(3)	-1(3)
C9	34(4)	48(4)	42(4)	-4(3)	5(3)	-12(3)
C10	42(4)	60(4)	27(4)	-2(3)	11(3)	-15(3)
C11	33(4)	26(3)	46(4)	-3(3)	11(3)	-2(3)
C12	37(4)	91(6)	69(5)	2(4)	17(4)	5(4)
C13	53(5)	95(6)	51(5)	8(4)	1(4)	16(4)

Table 4 Bond Lengths for Np2(1,4-bdc)4(DMF)4.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	O1	2.463(3)		N1	C11	1.308(7)
Np1	$O1^1$	2.463(3)		N1	C12	1.446(8)
Np1	$O2^2$	2.493(3)		N1	C13	1.464(8)
Np1	$O2^3$	2.493(3)		C1	$O1^1$	1.265(5)
Np1	$O3^1$	2.441(4)		C1	C2	1.505(10)
Np1	O3	2.441(4)		C2	C3	1.361(7)
Np1	O4	2.504(4)		C2	$C3^1$	1.361(7)
Np1	$O4^1$	2.504(4)		C3	C4	1.382(7)
Np1	O5	2.334(4)		C4	C5	1.402(7)
Np1	$O5^1$	2.334(4)		C5	$C4^1$	1.402(7)
Np1	C7	2.810(5)		C5	C6	1.530(10)
Np1	$C7^1$	2.810(5)		C6	$Np1^4$	2.820(7)
O1	C1	1.265(5)		C6	$O2^1$	1.224(5)
O2	$Np1^4$	2.493(3)		C7	C8	1.524(7)
O2	C6	1.224(5)		C8	C9	1.388(8)
O3	C7	1.217(6)		C8	$C10^5$	1.392(8)
O4	C7	1.222(6)		C9	C10	1.378(8)
O5	C11	1.231(7)		C10	$C8^5$	1.392(8)

[1]1-X,+Y,3/2-Z; [2]+X,-1+Y,+Z; [3]1-X,-1+Y,3/2-Z; [4]+X,1+Y,+Z; [5]3/2-X,1/2-Y,1-Z

II.34 Th-ndc

Table 1 Crystal data and structure refinement for Th-ndc.	
Identification code	Th-ndc
Empirical formula	$C_{144}O_{76}Th_{12}$
Formula weight	5729.92
Temperature/K	100.03
Crystal system	cubic
Space group	Fm-3m
a/Å	24.9499(17)
b/Å	24.9499(17)
c/Å	24.9499(17)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	15531(3)
Z	2
ρ_{calc}g/cm^3	1.225
μ/mm^{-1}	5.771
F(000)	5104.0
Crystal size/mm^3	0.12 × 0.011 × 0.01
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.828 to 52.726
Index ranges	-17 ≤ h ≤ 30, -24 ≤ k ≤ 28, -31 ≤ l ≤ 17
Reflections collected	9111
Independent reflections	862 [R_{int} = 0.0701, R_{sigma} = 0.0369]
Data/restraints/parameters	862/0/30
Goodness-of-fit on F^2	1.227
Final R indexes [I>=2σ (I)]	R_1 = 0.1095, wR_2 = 0.2994
Final R indexes [all data]	R_1 = 0.1258, wR_2 = 0.3110
Largest diff. peak/hole / e Å^{-3}	2.70/-2.99

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-ndc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	6117.0(6)	5000	5000	42.7(8)
O1	5509(12)	4491(12)	4491(12)	75(14)
O2	6539(14)	5884(13)	5000	104(9)
O1W	7220(30)	5000	5000	190(40)
C1	6330(30)	6330(30)	5000	140(30)
C4	7900(40)	6810(40)	5000	110(40)
C5	7760(30)	7390(40)	5000	90(20)
C3	7440(40)	6480(40)	5000	100(30)
C6	7210(30)	6830(30)	5000	63(17)
C2	6900(30)	6690(20)	5000	62(17)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Th-ndc. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka*b*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	11.2(9)	58.4(10)	58.4(10)	0	0	0
O1	75(14)	75(14)	75(14)	41(16)	-41(16)	-41(16)
O1W	50(40)	250(70)	250(70)	0	0	0

Table 4 Bond Lengths for Th-ndc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	Th1[1]	3.941(2)		C4	C3	1.42(13)
Th1	Th1[2]	3.941(2)		C4	C6	1.74(12)
Th1	Th1[3]	3.941(2)		C5	C4[10]	1.29(10)
Th1	O1[4]	2.351(13)		C5	C5[9]	1.31(13)
Th1	O1[5]	2.351(13)		C5	C5[10]	0.5(2)
Th1	O1	2.351(13)		C5	C5[11]	1.42(13)
Th1	O1[6]	2.351(13)		C5	C3[10]	1.95(13)
Th1	O2	2.44(3)		C5	C6	1.96(13)
Th1	O2[6]	2.44(3)		C5	C6[10]	1.43(12)
Th1	O2[7]	2.44(3)		C5	C6[11]	1.95(11)
Th1	O2[8]	2.44(3)		C3	C5[10]	1.95(13)
Th1	O1W	2.75(7)		C3	C6	1.06(10)
O1	Th1[3]	2.351(13)		C3	C2	1.44(11)
O1	Th1[1]	2.351(13)		C6	C5[11]	1.95(11)
O2	C1	1.23(5)		C6	C5[10]	1.43(12)
C1	O2[9]	1.23(5)		C6	C6[9]	1.33(14)
C1	C2[9]	1.68(11)		C6	C2	0.83(8)
C1	C2	1.68(11)		C6	C2[9]	1.31(8)
C4	C4[10]	1.0(2)		C2	C6[9]	1.31(8)
C4	C5	1.48(10)		C2	C2[9]	0.76(12)
C4	C5[10]	1.29(10)				

[1]1-Z,1-X,1-Y; [2]+Z,+X,+Y; [3]1-Y,1-Z,1-X; [4]+X,1-Y,1-Z; [5]+X,+Y,1-Z; [6]+X,1-Y,+Z; [7]+X,+Z,1-Y; [8]+X,+Z,+Y; [9]+Y,+X,1-Z; [10]3/2-Y,3/2-X,+Z; [11]3/2-X,3/2-Y,1-Z

II.35 Th-bpdc

Table 1 Crystal data and structure refinement for Th-bpdc.

Identification code	Th-bpdc
Empirical formula	$C_{168}O_{70}Th_{12}$
Formula weight	5922.16
Temperature/K	296.15
Crystal system	cubic
Space group	Fm-3m
a/Å	27.9879(11)

b/Å	27.9879(11)
c/Å	27.9879(11)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	21924(3)
Z	2
ρ_{calc}g/cm^3	0.897
μ/mm^{-1}	4.089
F(000)	5296.0
Crystal size/mm^3	0.094 × 0.092 × 0.055
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.52 to 52.654
Index ranges	-12 ≤ h ≤ 34, -31 ≤ k ≤ 21, -11 ≤ l ≤ 34
Reflections collected	11372
Independent reflections	1177 [R_{int} = 0.1213, R_{sigma} = 0.0577]
Data/restraints/parameters	1177/0/42
Goodness-of-fit on F^2	1.255
Final R indexes [I>=2σ (I)]	R_1 = 0.0623, wR_2 = 0.1955
Final R indexes [all data]	R_1 = 0.0902, wR_2 = 0.2100
Largest diff. peak/hole / e Å^{-3}	1.74/-1.84

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-bpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	5000	3997.2(3)	5000	21.8(4)
O2	4199(4)	3632(4)	5000	55(4)
C5	3776(6)	3776(6)	5000	49(7)
C1	3400(6)	3400(6)	5000	60(8)
C4	2693(8)	2693(8)	5000	76(9)
O1B	5536(11)	4464(11)	4464(11)	25(11)
C2B	3513(14)	2923(14)	5000	46(9)
C3B	3166(13)	2566(13)	5000	42(8)
O1A	5398(12)	4602(12)	4602(12)	19(13)
C3A	3110(20)	2600(20)	5265(19)	55(14)
C2A	3470(20)	3000(20)	5240(20)	58(15)
O1W	5000	3040(13)	5000	39(11)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Th-bpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	24.4(5)	16.6(6)	24.4(5)	0	0	0
O2	36(7)	39(7)	92(11)	0	0	-23(6)
C5	43(10)	43(10)	60(17)	0	0	-25(13)
C1	37(9)	37(9)	110(30)	0	0	-15(12)
O1W	57(18)	3(17)	57(18)	0	0	0

Table 4 Bond Lengths for Th-bpdc.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Th1	O2	2.465(11)		C1	C2A^{6}	1.33(6)
Th1	O2^{1}	2.465(11)		C1	C2A^{7}	1.33(6)
Th1	O2^{2}	2.465(11)		C4	C4^{8}	1.53(6)
Th1	O2^{3}	2.465(11)		C4	C3B^{6}	1.37(4)
Th1	O1B^{4}	2.49(2)		C4	C3B	1.37(4)
Th1	O1B	2.49(2)		C4	C3A^{6}	1.41(6)
Th1	O1B^{5}	2.49(2)		C4	C3A^{4}	1.41(6)
Th1	O1B^{3}	2.49(2)		C4	C3A	1.41(6)
Th1	O1A	2.313(8)		C4	C3A^{7}	1.41(6)
Th1	O1A^{5}	2.313(8)		O1B	Th1^{9}	2.49(2)
Th1	O1A^{4}	2.313(8)		O1B	Th1^{10}	2.49(2)
Th1	O1A^{3}	2.313(8)		C2B	C3B	1.39(5)
Th1	O1W	2.68(4)		O1A	Th1^{9}	2.313(8)
O2	C5	1.250(16)		O1A	Th1^{10}	2.313(8)
C5	O2^{6}	1.250(16)		C3A	C3A^{7}	2.03(11)
C5	C1	1.49(3)		C3A	C3A^{4}	1.48(11)
C1	C2B^{6}	1.37(4)		C3A	C2A	1.51(9)
C1	C2B	1.37(4)		C2A	C2A^{7}	1.89(12)
C1	C2A^{4}	1.33(6)		C2A	C2A^{4}	1.36(12)
C1	C2A	1.33(6)				

^{1}+Z,+Y,1-X; ^{2}1-Z,+Y,+X; ^{3}1-X,+Y,1-Z; ^{4}+X,+Y,1-Z; ^{5}1-X,+Y,+Z; ^{6}+Y,+X,1-Z; ^{7}+Y,+X,+Z; ^{8}1/2-X,1/2-Y,1-Z; ^{9}1-Y,1-Z,1-X; ^{10}+Z,+X,+Y

II.36 Th-NH_2-bpdc

Table 1 Crystal data and structure refinement for Th-NH2-bpdc.	
Identification code	Th-NH2-bpdc
Empirical formula	$C_{168}O_{70}Th_{12}$
Formula weight	5922.16
Temperature/K	299.18
Crystal system	cubic
Space group	Fm-3m
a/Å	27.9960(15)
b/Å	27.9960(15)
c/Å	27.9960(15)
α/°	90
β/°	90
γ/°	90
Volume/Å^{3}	21943(4)
Z	2
ρ_{calc}g/cm^{3}	0.896
μ/mm^{-1}	4.085
F(000)	5296.0

Crystal size/mm^3	0.162 × 0.158 × 0.141
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.52 to 60.858
Index ranges	-33 ≤ h ≤ 39, -39 ≤ k ≤ 30, -27 ≤ l ≤ 39
Reflections collected	40250
Independent reflections	1704 [R_{int} = 0.0686, R_{sigma} = 0.0233]
Data/restraints/parameters	1704/0/41
Goodness-of-fit on F^2	1.302
Final R indexes [I>=2σ (I)]	R_1 = 0.0445, wR_2 = 0.1371
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1508
Largest diff. peak/hole / e Å^{-3}	2.45/-1.68

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-NH2-bpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	5000	3996.8(2)	5000	20.57(18)
O2	4202(2)	3632(2)	5000	59.2(19)
C5	3774(3)	3774(3)	5000	51(3)
C1	3394(3)	3394(3)	5000	65(4)
C4	2686(5)	2686(5)	5000	90(6)
O1B	5540(4)	4460(4)	4460(4)	15(4)
C2B	3502(9)	2933(9)	5000	64(6)
C3B	3144(10)	2573(10)	5000	71(6)
O1A	5398(4)	4602(4)	4602(4)	19(4)
C3A	3115(12)	2601(12)	5276(11)	60(7)
C2A	3476(10)	2966(10)	5259(9)	46(5)
O1W	5000	3037(9)	5000	47(6)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Th-NH2-bpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	23.5(2)	14.8(2)	23.5(2)	0	0	0
O2	44(4)	38(3)	96(6)	0	0	-25(3)
C5	44(5)	44(5)	67(9)	0	0	-32(6)
C1	40(4)	40(4)	116(14)	0	0	-20(6)

Table 4 Bond Lengths for Th-NH2-bpdc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	Th1^1	3.9717(6)		C1	C2A^8	1.42(3)
Th1	O2^2	2.456(6)		C1	C2A^6	1.42(3)
Th1	O2	2.456(6)		C1	C2A	1.42(3)
Th1	O2^3	2.456(6)		C4	C4^9	1.47(4)
Th1	O2^4	2.456(6)		C4	C3B	1.32(3)
Th1	O1B^5	2.500(8)		C4	C3B^7	1.32(3)

Th1	O1B^{6}	2.500(8)		C4	C3A^{6}	1.45(3)
Th1	O1B	2.500(8)		C4	C3A^{7}	1.45(3)
Th1	O1B^{4}	2.500(8)		C4	C3A	1.45(3)
Th1	O1A^{6}	2.314(3)		C4	C3A^{8}	1.45(3)
Th1	O1A	2.314(3)		O1B	Th1^{10}	2.500(8)
Th1	O1A^{5}	2.314(3)		O1B	Th1^{11}	2.500(8)
Th1	O1A^{4}	2.314(3)		C2B	C3B	1.42(4)
Th1	O1W	2.69(3)		O1A	Th1^{10}	2.314(3)
O2	C5	1.261(9)		O1A	Th1^{11}	2.314(3)
C5	O2^{7}	1.261(9)		C3A	C3A^{6}	1.55(6)
C5	C1	1.507(16)		C3A	C3A^{8}	2.04(6)
C1	C2B^{7}	1.32(3)		C3A	C2A	1.44(4)
C1	C2B	1.32(3)		C2A	C2A^{6}	1.45(5)
C1	C2A^{7}	1.42(3)		C2A	C2A^{8}	2.02(5)

^{1}1-Z,1-X,1-Y; ^{2}+Z,+Y,1-X; ^{3}1-Z,+Y,+X; ^{4}1-X,+Y,1-Z; ^{5}1-X,+Y,+Z; ^{6}+X,+Y,1-Z; ^{7}+Y,+X,1-Z; ^{8}+Y,+X,+Z; ^{9}1/2-X,1/2-Y,1-Z; ^{10}1-Y,1-Z,1-X; ^{11}+Z,+X,+Y

II.37 Th-NH_2-tpdc

Table 1 Crystal data and structure refinement for Th-NH2-tpdc.	
Identification code	Th-NH2-tpdc
Empirical formula	$C_{240}O_{76}Th_{12}$
Formula weight	6882.88
Temperature/K	296.15
Crystal system	cubic
Space group	Fm-3m
a/Å	33.986(3)
b/Å	33.986(3)
c/Å	33.986(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	39255(10)
Z	2
ρ_{calc}g/cm^3	0.582
μ/mm^{-1}	2.289
F(000)	6256.0
Crystal size/mm^3	0.223 × 0.122 × 0.105
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.396 to 46.48
Index ranges	-37 ≤ h ≤ 36, -37 ≤ k ≤ 35, -35 ≤ l ≤ 36
Reflections collected	43728
Independent reflections	1459 [R_{int} = 0.0990, R_{sigma} = 0.0305]
Data/restraints/parameters	1459/9/28
Goodness-of-fit on F^2	1.113
Final R indexes [I>=2σ (I)]	R_1 = 0.0717, wR_2 = 0.2243

Final R indexes [all data]	R_1 = 0.0905, wR_2 = 0.2456
Largest diff. peak/hole / e Å^{-3}	2.59/-2.56

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Th-NH2-tpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Th1	5000	5822.1(3)	5000	42.6(5)
O1B	4546(7)	5454(7)	4546(7)	53(11)
O3	5000	6133(5)	5662(5)	119(6)
C1	5000	6003(5)	6003(5)	109(11)
O1W	5000	6622(16)	5000	240(30)
C2	5000	6316(6)	6316(6)	100
C3	5000	6195(6)	6712(5)	100
C4	5000	6486(5)	7007(6)	100
C5	5000	6882(4)	6882(4)	100
O1A	4659(6)	5341(6)	4659(6)	32(7)
C7	5000	7071(6)	7594(5)	100
C6	5000	7197(4)	7197(4)	100

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Th-NH2-tpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Th1	57.7(6)	12.3(6)	57.7(6)	0	0	0
O3	172(17)	77(10)	107(13)	-66(10)	0	0
O1W	310(50)	120(40)	310(50)	0	0	0

Table 4 Bond Lengths for Th-NH2-tpdc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Th1	O1B	2.515(18)		O3	C1	1.24(2)
Th1	O1B^1	2.515(18)		C1	O3^8	1.24(2)
Th1	O1B^2	2.515(18)		C1	C2	1.507(18)
Th1	O1B^3	2.515(18)		C2	C3	1.406(14)
Th1	O3^4	2.485(14)		C2	C3^8	1.406(14)
Th1	O3	2.485(14)		C3	C4	1.409(16)
Th1	O3^1	2.485(14)		C4	C5	1.411(14)
Th1	O3^5	2.485(14)		C5	C4^8	1.411(14)
Th1	O1W	2.72(5)		C5	C6	1.515(17)
Th1	O1A^1	2.315(6)		O1A	Th1^6	2.315(6)
Th1	O1A^3	2.315(6)		O1A	Th1^7	2.315(6)
Th1	O1A	2.315(6)		C7	C7^9	1.61(4)
Th1	O1A^2	2.315(6)		C7	C6	1.414(14)
O1B	Th1^6	2.515(18)		C6	C7^8	1.414(14)
O1B	Th1^7	2.515(18)				

[1]+X,+Y,1-Z; [2]1-X,+Y,+Z; [3]1-X,+Y,1-Z; [4]+Z,+Y,1-X; [5]1-Z,+Y,1-X; [6]1-Y,1-Z,1-X; [7]1-Z,1-X,1-Y; [8]1-X,+Z,+Y; [9]+X,3/2-Z,3/2-Y

II.38 Np-ndc

Table 1 Crystal data and structure refinement for Np-ndc.	
Identification code	Th-bpdc
Empirical formula	Np36 O219 C432
Formula weight	17226.26
Temperature/K	100
Crystal system	trigonal
Space group	R -3
a/Å	34.8219(4)
b/Å	34.8219(4)
c/Å	42.6479(4)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	44785.1(9)
Z	2
ρ_{calc}g/cm^3	1.2774
μ/mm^{-1}	4.186
F(000)	15384
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.34 to 30.57
Index ranges	-48 ≤ h ≤ 48, -44 ≤ k ≤ 48, -60 ≤ l ≤ 60
Reflections collected	263276
Independent reflections	22252 [R_{int} = 0.0339, R_{sigma} = 0.0159]
Data/restraints/parameters	22252/ 288/ 26
Goodness-of-fit on F^2	7.99
Final R indexes [I>=2σ (I)]	R_1 = 0.0467, wR_2 = 0.1093
Final R indexes [all data]	R_1 = 0.0467, wR_2 = 0.1093
Largest diff. peak/hole / e Å^{-3}	8.07 / -3.89

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np-ndc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	0.0292(2)	0.07474(17)	0.46602(12)	-0.0074(10)
Np2	-0.13930(19)	-0.26070(18)	0.12781(11)	-0.0064(8)
Np3	-0.20030(14)	0.09388(17)	0.20339(15)	-0.0046(7)
Np4	0.30708(15)	0.10044(17)	0.20200(13)	0.0017(9)
O12d	0.3211	0.0387	0.1848	0.0327(8)
O82c	-0.1545	-0.2054	0.1485	0.0327(8)
O82d	0.0122	0.128	0.4819	0.0327(8)
O12c	-0.1797	0.0375	0.1848	0.0327(8)

O12a	-0.1474	0.1001	0.2463	0.0327(8)
O82a	-0.0205	0.067	0.4203	0.0327(8)
O12b	-0.1869	-0.2663	0.087	0.0327(8)
O82b	0.3537	0.0997	0.2463	0.0327(8)
O11c	-0.1378	0.063	0.1455	0.0327(8)
O11d	0.3623	0.063	0.1455	0.0327(8)
O81c	-0.1954	-0.2296	0.1878	0.0327(8)
O81d	-0.029	0.1037	0.5211	0.0327(8)
O11a	-0.0919	0.1648	0.2474	0.0327(8)
O81b	0.406	0.1645	0.2474	0.0327(8)
O81a	-0.0724	0.0024	0.4193	0.0327(8)
O11b	-0.2392	-0.331	0.086	0.0327(8)
O1	0.2595	0.1231	0.1859	0.0327(8)
O2	-0.2079	-0.3021	0.1474	0.0327(8)
O3	-0.0412	0.0312	0.4807	0.0327(8)
O4	0.3745	0.1355	0.1859	0.0327(8)
C7d	0.3256	-0.1556	0.1743	0.0455(12)
C7b	0.4024	0.1155	0.2857	0.0455(12)
C2d	0.3432	-0.009	0.1589	0.0455(12)
C7a	-0.0694	0.051	0.3811	0.0455(12)
C7c	-0.175	-0.1584	0.1744	0.0455(12)
C2c	-0.1584	-0.0084	0.1589	0.0455(12)
C2b	0.4308	0.051	0.3811	0.0455(12)
C2a	-0.098	0.1164	0.2855	0.0455(12)
C6a	-0.0476	0.0858	0.3654	0.0455(12)
C6b	0.381	0.0809	0.3013	0.0455(12)
C12a	-0.1203	0.0799	0.3012	0.0455(12)
C12b	0.4524	0.0858	0.3654	0.0455(12)
C6d	0.3425	-0.1267	0.152	0.0455(12)
C12c	-0.1778	-0.0409	0.1814	0.0455(12)
C6c	-0.1553	-0.1255	0.1517	0.0455(12)
C12d	0.3239	-0.0414	0.1816	0.0455(12)
C5d	0.3435	-0.0818	0.1553	0.0455(12)
C11d	0.322	-0.0841	0.1781	0.0455(12)
C11c	-0.1769	-0.0831	0.178	0.0455(12)
C5c	-0.1565	-0.0838	0.1553	0.0455(12)
C5a	-0.0633	0.0979	0.3372	0.0455(12)
C11a	-0.1037	0.0686	0.3294	0.0455(12)
C5b	0.3966	0.0687	0.3292	0.0455(12)
C11b	0.4367	0.098	0.3374	0.0455(12)
C1d	0.3403	0.0344	0.1659	0.0455(12)
C8c	-0.1763	-0.2035	0.1681	0.0455(12)
C1c	-0.1543	0.0385	0.1655	0.0455(12)
C8d	-0.0127	0.1282	0.5013	0.0455(12)
C3d	0.3642	-0.0141	0.134	0.0455(12)
C4d	0.3648	-0.0506	0.1311	0.0455(12)
C10d	0.302	-0.1179	0.2039	0.0455(12)
C9d	0.3014	-0.1526	0.2025	0.0455(12)

C9b	0.4493	0.1482	0.2969	0.0455(12)
C10b	0.4652	0.1387	0.3224	0.0455(12)
C4b	0.3674	0.0273	0.3444	0.0455(12)
C3b	0.3847	0.0186	0.3704	0.0455(12)
C1b	0.4418	0.0362	0.4075	0.0455(12)
C8b	0.3929	0.129	0.2623	0.0455(12)
C9c	-0.1985	-0.1557	0.1971	0.0455(12)
C10c	-0.199	-0.116	0.2013	0.0455(12)
C4c	-0.1308	-0.0485	0.1314	0.0455(12)
C3c	-0.1317	-0.0107	0.1359	0.0455(12)
C9a	-0.1164	0.0184	0.3705	0.0455(12)
C10a	-0.1327	0.031	0.3419	0.0455(12)
C4a	-0.0336	0.142	0.32	0.0455(12)
C3a	-0.0517	0.1484	0.2961	0.0455(12)
C1a	-0.1108	0.1272	0.2621	0.0455(12)
O6	0	0	0.457	0.0327(8)
C8a	-0.0523	0.0437	0.405	0.0455(12)
O5	-0.1668	-0.3361	0.1231	0.0327(8)
O4w	-0.0228	0.2421	0.2401	0.0327(8)
O2w	0.4772	0.2421	0.2401	0.0327(8)
O3w	-0.3108	-0.4083	0.0932	0.0327(8)

Table 3 Bond Lengths for Np-ndc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	O82d	2.311(8)		C7b	C6b	1.24711(3)
Np1	O82a	2.530(6)		C7b	C5b	2.41108(4)
Np1	O81d^i^	2.423(5)		C7b	C11b	2.71816(4)
Np1	O81a^ii^	2.576(7)		C7b	C9b	1.52662(5)
Np1	O3	2.232(6)		C7b	C10b	2.47418(5)
Np1	O3^ii^	2.405(8)		C7b	C8b	1.216337(16)
Np1	O3^i^	2.275(5)		C2d	C12d	1.37775(3)
Np1	O6	2.304(6)		C2d	C5d	2.54423(6)
Np2	O82c	2.403(7)		C2d	C11d	2.47415(7)
Np2	O12b	2.344(6)		C2d	C1d	1.59135(3)
Np2	O11c^iii^	2.537(5)		C2d	C3d	1.352279(18)
Np2	O81b^iv^	2.435(6)		C2d	C4d	2.27045(3)
Np2	O1^ii^	2.480(5)		C7a	C6a	1.25541(3)
Np2	O2	2.244(5)		C7a	C5a	2.42257(4)
Np2	O4^iv^	2.464(8)		C7a	C11a	2.72015(4)
Np2	O5	2.311(6)		C7a	C9a	1.52034(5)
Np2	O2w^iv^	2.614(5)		C7a	C10a	2.56886(5)
Np3	O12c	2.533(7)		C7a	C8a	1.266276(17)
Np3	O12a	2.527(6)		C7c	C6c	1.39096(3)
Np3	O11d^v^	2.377(4)		C7c	C11c	2.66210(6)
Np3	O11b^vi^	2.363(6)		C7c	C5c	2.48240(6)
Np3	O1^iii^	2.449(4)		C7c	C8c	1.57051(4)

Np3	O2^vi^	2.252(7)		C7c	C9c	1.300619(18)
Np3	O4^v^	2.389(6)		C7c	C10c	2.32957(3)
Np3	O5^vi^	2.209(5)		C2c	C12c	1.37806(3)
Np3	O3w^vi^	2.662(6)		C2c	C11c	2.48205(6)
Np4	O12d	2.538(7)		C2c	C5c	2.66257(6)
Np4	O82b	2.502(6)		C2c	C1c	1.58976(4)
Np4	O81c^iii^	2.597(4)		C2c	C4c	2.36519(3)
Np4	O11a^ii^	2.529(6)		C2c	C3c	1.380982(19)
Np4	O1	2.266(6)		C2b	C12b	1.25398(3)
Np4	O2^iii^	2.336(6)		C2b	C5b	2.72675(4)
Np4	O4	2.146(5)		C2b	C11b	2.42012(4)
Np4	O5^vii^	1.971(5)		C2b	C4b	2.48628(5)
Np4	O4w^ii^	2.854(5)		C2b	C3b	1.49864(5)
O12d	O11d	2.09168(4)		C2b	C1b	1.371620(18)
O12d	O2^iii^	2.82789(4)		C2a	C12a	1.29521(4)
O12d	O4	2.92376(10)		C2a	C5a	2.74266(4)
O12d	C2d	2.42014(3)		C2a	C11a	2.44656(4)
O12d	C12d	2.84214(6)		C2a	C4a	2.44710(5)
O12d	C1d	1.106249(15)		C2a	C3a	1.50037(5)
O12d	O4w^ii^	2.93640(5)		C2a	C1a	1.226707(16)
O82c	O81c	2.08633(4)		C6a	C5a	1.46537(2)
O82c	O1^ii^	2.77094(4)		C6a	C11a	2.31519(4)
O82c	O2	2.92191(10)		C6a	C9a	2.38171(9)
O82c	C7c	2.36307(3)		C6a	C10a	2.78712(9)
O82c	C6c	2.80076(6)		C6a	C4a	2.62048(4)
O82c	C8c	1.155134(16)		C6a	C8a	2.18725(3)
O82c	O2w^iv^	2.93562(5)		C6b	C5b	1.456668(19)
O82d	O81d	2.08502(4)		C6b	C11b	2.30960(4)
O82d	O3	2.92217(10)		C6b	C9b	2.36915(9)
O82d	O3^i^	2.82965(4)		C6b	C10b	2.74986(9)
O82d	C7d^viii^	2.42574(3)		C6b	C4b	2.49151(4)
O82d	C6d^viii^	2.79663(6)		C6b	C8b	2.24661(4)
O82d	C8d	1.199513(18)		C12a	C5a	2.33581(4)
O12c	O11c	2.10515(4)		C12a	C11a	1.47199(2)
O12c	O1^iii^	2.99630(11)		C12a	C10a	2.31889(4)
O12c	O4^v^	2.84969(4)		C12a	C4a	2.81256(10)
O12c	C2c	2.34538(3)		C12a	C3a	2.39750(9)
O12c	C12c	2.76646(6)		C12a	C1a	2.24787(4)
O12c	C1c	1.196706(18)		C12b	C5b	2.31624(4)
O12c	O3w^vi^	2.94012(5)		C12b	C11b	1.462257(19)
O12a	O11a	2.11041(8)		C12b	C10b	2.47425(4)
O12a	O1^iii^	2.80629(5)		C12b	C4b	2.77281(9)
O12a	C2a	2.25834(4)		C12b	C3b	2.35922(9)
O12a	C12a	2.74342(4)		C12b	C1b	2.39034(4)
O12a	C1a	1.32751(4)		C6d	C5d	1.55297(4)
O12a	O3w^vi^	2.92137(11)		C6d	C11d	2.23683(3)
O82a	O81a	2.06325(8)		C6d	C8d^xii^	2.53307(7)
O82a	O3	2.79522(5)		C6d	C4d	2.52508(7)

O82a	C7a	2.24984(4)		C6d	C10d	2.72162(4)
O82a	C6a	2.72617(4)		C6d	C9d	2.48928(4)
O82a	C8a	1.19028(3)		C12c	C11c	1.49085(3)
O12b	O11b	2.07033(8)		C12c	C5c	2.26353(3)
O12b	O2	2.79505(5)		C12c	C1c	2.55229(7)
O12b	C2b^ix^	2.25121(4)		C12c	C10c	2.48265(7)
O12b	C12b^ix^	2.72973(4)		C12c	C4c	2.78157(4)
O12b	C1b^ix^	1.33400(4)		C12c	C3c	2.40262(4)
O12b	O2w^iv^	2.91813(11)		C6c	C11c	2.26126(3)
O82b	O81b	2.07358(8)		C6c	C5c	1.48310(3)
O82b	O4	2.79495(5)		C6c	C8c	2.53196(7)
O82b	C7b	2.24886(4)		C6c	C9c	2.35254(4)
O82b	C6b	2.72720(4)		C6c	C10c	2.71933(4)
O82b	C8b	1.40414(4)		C6c	C4c	2.52553(7)
O82b	O4w^ii^	2.92186(11)		C12d	C5d	2.16132(3)
O11c	O1^iii^	2.90925(6)		C12d	C11d	1.46503(3)
O11c	O4^v^	2.80211(4)		C12d	C1d	2.49365(7)
O11c	C2c	2.28955(6)		C12d	C3d	2.38036(4)
O11c	C1c	1.13836(2)		C12d	C4d	2.68916(4)
O11c	C3c	2.70886(6)		C12d	C10d	2.55810(7)
O11c	O2w^v^	2.66710(5)		C5d	C11d	1.205318(18)
O11d	O2^iii^	2.80529(4)		C5d	C3d	2.28101(6)
O11d	O4	2.90714(5)		C5d	C4d	1.41187(3)
O11d	C2d	2.32232(6)		C5d	C10d	2.47818(4)
O11d	C1d	1.25545(3)		C5d	C9d	2.94322(6)
O11d	C3d	2.76276(6)		C11d	C3d	2.83939(6)
O11d	O3w^iii^	2.65662(5)		C11d	C4d	2.42217(4)
O81c	O1^ii^	2.72761(4)		C11d	C10d	1.50097(3)
O81c	O2	2.90556(5)		C11d	C9d	2.36059(6)
O81c	C7c	2.28273(6)		C11c	C5c	1.205542(17)
O81c	C8c	1.17036(2)		C11c	C9c	2.39435(6)
O81c	C9c	2.65756(6)		C11c	C10c	1.41921(3)
O81c	O4w^iii^	2.67069(5)		C11c	C4c	2.45602(4)
O81d	O3	2.90403(5)		C11c	C3c	2.84318(7)
O81d	O3^i^	2.80613(4)		C5c	C9c	2.81597(7)
O81d	C7d^viii^	2.36836(7)		C5c	C10c	2.37241(4)
O81d	C8d	1.13050(2)		C5c	C4c	1.49957(3)
O81d	C9d^viii^	2.80589(6)		C5c	C3c	2.39060(7)
O11a	O1^iii^	2.81937(5)		C5a	C11a	1.30291(5)
O11a	C2a	2.27223(4)		C5a	C9a	2.82505(8)
O11a	C3a	2.71918(3)		C5a	C10a	2.38331(9)
O11a	C1a	1.29522(4)		C5a	C4a	1.54407(5)
O11a	O5^vi^	2.99714(5)		C5a	C3a	2.37145(4)
O11a	O4w	2.57954(10)		C11a	C9a	2.35696(4)
O81b	O4	2.82724(5)		C11a	C10a	1.30323(4)
O81b	C7b	2.31690(4)		C11a	C4a	2.53388(10)
O81b	C9b	2.81026(4)		C11a	C3a	2.82669(8)
O81b	C8b	1.25455(3)		C5b	C11b	1.30044(5)

O81b	O2w	2.61547(10)		C5b	C9b	2.80189(8)
O81a	O3	2.82327(5)		C5b	C10b	2.43126(9)
O81a	C7a	2.31173(4)		C5b	C4b	1.43742(4)
O81a	C9a	2.79894(4)		C5b	C3b	2.36252(4)
O81a	C8a	1.38671(4)		C11b	C9b	2.33706(4)
O11b	O2	2.82086(5)		C11b	C10b	1.41159(4)
O11b	C2b^ix^	2.31392(4)		C11b	C4b	2.45619(10)
O11b	C3b^ix^	2.78243(4)		C11b	C3b	2.81015(8)
O11b	C1b^ix^	1.14198(3)		C1d	C3d	2.60756(3)
O11b	O3w	2.61784(10)		C8c	C9c	2.48610(3)
O1	O2^iii^	2.71867(3)		C1c	C3c	2.54549(3)
O1	O4^x^	2.79562(6)		C8d	C9d^viii^	2.68138(3)
O1	O5^vii^	2.38578(7)		C3d	C4d	1.28532(3)
O2	O4^ii^	2.73656(6)		C10d	C9d	1.20253(3)
O2	O5	2.49059(3)		C9b	C10b	1.335909(18)
O3	O3^i^	2.73848(7)		C9b	C8b	2.27366(5)
O3	O3^xi^	2.73848(6)		C4b	C3b	1.366289(18)
O3	O6	2.41362(3)		C3b	C1b	2.36971(4)
O4	O5^vii^	2.43430(3)		C9c	C10c	1.40352(3)
C7d	C6d	1.29118(3)		C4c	C3c	1.34814(3)
C7d	C5d	2.45980(6)		C9a	C10a	1.50011(2)
C7d	C11d	2.56032(6)		C9a	C8a	2.43813(5)
C7d	C8d^xii^	1.66659(4)		C4a	C3a	1.274037(17)
C7d	C10d	2.25459(3)		C3a	C1a	2.31730(5)
C7d	C9d	1.50181(2)				

(i) y,-x+y,-z+1 ; (ii) -x+y,-x,z ; (iii) -y,x-y,z ; (iv) x-y-1/3,x-2/3,-z+1/3 ; (v) y-1/3,-x+y+1/3,-z+1/3 ; (vi) x-y-1/3,x+1/3,-z+1/3 ; (vii) y+2/3,-x+y+1/3,-z+1/3 ; (viii) x-1/3,y+1/3,z+1/3 ; (ix) x-2/3,y-1/3,z-1/3 ; (x) -x+2/3,-y+1/3,-z+1/3 ; (xi) x-y,x,-z+1 ; (xii) x+1/3,y-1/3,z-1/3

II.39 Np-bpdc

Table 1 Crystal data and structure refinement for Np-bpdc.	
Identification code	Th-bpdc
Empirical formula	$C_{336}Np_{24}O_{184}$
Formula weight	12668.37
Temperature/K	100.25
Crystal system	cubic
Space group	Fm-3m
a/Å	27.6042(12)
b/Å	27.6042(12)
c/Å	27.6042(12)
α/°	90
β/°	90
γ/°	90

Volume/Å^3	21034(3)
Z	1
ρ_{calc}g/cm^3	1.000
μ/mm^{-1}	2.979
F(000)	5721.0
Crystal size/mm^3	0.328 × 0.242 × 0.233
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.894 to 61.014
Index ranges	-38 ≤ h ≤ 38, -35 ≤ k ≤ 38, -39 ≤ l ≤ 34
Reflections collected	59776
Independent reflections	1642 [R_{int} = 0.0291, R_{sigma} = 0.0074]
Data/restraints/parameters	1642/0/45
Goodness-of-fit on F^2	1.248
Final R indexes [I>=2σ (I)]	R_1 = 0.0321, wR_2 = 0.1081
Final R indexes [all data]	R_1 = 0.0348, wR_2 = 0.1114
Largest diff. peak/hole / e Å^{-3}	2.47/-1.72

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np-bpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	5000	4032.2(2)	5000	8.94(13)
O1L	4226.5(16)	3640.8(16)	5000	33.5(10)
C5	3792.8(18)	3792.8(18)	5000	32.6(18)
C1	3408(2)	3408(2)	5000	46(3)
C4	2689(3)	2689(3)	5000	59(3)
O1B	5540(3)	4460(3)	4460(3)	13(3)
C2B	3538(5)	2914(5)	5000	36(3)
C3B	3178(6)	2560(6)	5000	42(3)
O1W	5000	3055(11)	5000	177(12)
O2W	6198(7)	3802(7)	3802(7)	194(12)
O1A	5400(3)	4600(3)	4600(3)	10(3)
C3A	3161(7)	2588(7)	5225(7)	32(3)
C2A	3522(6)	2941(6)	5209(6)	29(3)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for Np-bpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	10.50(14)	5.81(16)	10.50(14)	0	0	0
O1L	27(2)	25(2)	48(3)	0	0	-18.4(17)
C5	25(3)	25(3)	47(5)	0	0	-22(3)
C1	26(3)	26(3)	86(8)	0	0	-19(3)
O1W	190(19)	150(30)	190(19)	0	0	0

Table 4 Bond Lengths for Np-bpdc.						
Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Np1	O1L	2.393(4)		C1	C2A^{7}	1.447(18)
Np1	O1L^{1}	2.393(4)		C1	C2A^{6}	1.447(18)
Np1	O1L^{2}	2.393(4)		C4	C4^{8}	1.47(3)
Np1	O1L^{3}	2.393(4)		C4	C3B^{6}	1.396(17)
Np1	O1B^{4}	2.416(6)		C4	C3B	1.396(17)
Np1	O1B^{5}	2.416(6)		C4	C3A	1.47(2)
Np1	O1B^{3}	2.416(6)		C4	C3A^{4}	1.47(2)
Np1	O1B	2.416(6)		C4	C3A^{7}	1.47(2)
Np1	O1A^{4}	2.212(2)		C4	C3A^{6}	1.47(2)
Np1	O1A^{3}	2.212(2)		O1B	Np1^{9}	2.416(6)
Np1	O1A	2.212(2)		O1B	Np1^{10}	2.416(6)
Np1	O1A^{5}	2.212(2)		C2B	C3B	1.39(2)
O1L	C5	1.268(6)		O1A	Np1^{9}	2.212(2)
C5	O1L^{6}	1.268(6)		O1A	Np1^{10}	2.212(2)
C5	C1	1.501(11)		C3A	C3A^{4}	1.24(4)
C1	C2B	1.411(15)		C3A	C2A	1.39(2)
C1	C2B^{6}	1.411(15)		C3A	C2A^{4}	1.84(3)
C1	C2A	1.447(18)		C2A	C3A^{4}	1.84(2)
C1	C2A^{4}	1.447(18)		C2A	C2A^{4}	1.15(4)

^{1}1-Z,+Y,+X; ^{2}+Z,+Y,1-X; ^{3}1-X,+Y,1-Z; ^{4}+X,+Y,1-Z; ^{5}1-X,+Y,+Z; ^{6}+Y,+X,1-Z; ^{7}+Y,+X,+Z; ^{8}1/2-X,1/2-Y,1-Z; ^{9}1-Y,1-Z,1-X; ^{10}+Z,+X,+Y

II.40 Np-NH_2-bpdc

Table 1 Crystal data and structure refinement for Np-NH2-bpdc.	
Identification code	Np-NH2-bpdc
Empirical formula	$C_{168}Np_{12}O_{86}$
Formula weight	6237.68
Temperature/K	100.0
Crystal system	cubic
Space group	Fm-3m
a/Å	27.5467(12)
b/Å	27.5467(12)
c/Å	27.5467(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^{3}	20903(3)
Z	2
ρ_{calc}g/cm^{3}	0.991
μ/mm^{-1}	2.996
F(000)	5624.0
Crystal size/mm^{3}	? × ? × ?
Radiation	MoKα (λ = 0.71073)

2Θ range for data collection/°	4.182 to 52.706
Index ranges	$-33 \leq h \leq 34$, $-34 \leq k \leq 27$, $-34 \leq l \leq 34$
Reflections collected	47337
Independent reflections	1127 [R_{int} = 0.0360, R_{sigma} = 0.0079]
Data/restraints/parameters	1127/0/39
Goodness-of-fit on F^2	1.259
Final R indexes [I>=2σ (I)]	R_1 = 0.0352, wR_2 = 0.1178
Final R indexes [all data]	R_1 = 0.0380, wR_2 = 0.1212
Largest diff. peak/hole / e $Å^{-3}$	1.63/-1.75

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Np-NH2-bpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	5000	4031.4(2)	5000	10.4(2)
O2	5000	3642(2)	4225(2)	39.2(14)
O1B	4462(5)	4462(5)	4462(5)	11(5)
C1	5000	3792(3)	3792(3)	40(3)
C2	5000	3409(3)	3409(3)	56(4)
O1W	5000	3071(11)	5000	69(9)
O1A	4605(4)	4605(4)	4605(4)	9(5)
C5	5000	2682(5)	2682(5)	76(5)
C3	5158(5)	3521(6)	2935(6)	61(4)
C4	5162(6)	3145(6)	2579(6)	71(5)
O2W	3798(10)	3798(10)	3798(10)	219(18)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for Np-NH2-bpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	13.1(2)	5.1(3)	13.1(2)	0	0	0
O2	58(4)	28(3)	32(3)	-24(3)	0	0
C1	52(8)	34(4)	34(4)	-27(6)	0	0
C2	98(12)	35(5)	35(5)	-30(6)	0	0
O1W	85(15)	36(16)	85(15)	0	0	0
O2W	219(18)	219(18)	219(18)	90(20)	90(20)	90(20)

Table 4 Bond Lengths for Np-NH2-bpdc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	$Np1^1$	3.7735(6)		C1	C2	1.491(14)
Np1	$O2^2$	2.389(5)		C2	$C3^5$	1.412(16)
Np1	O2	2.389(5)		C2	$C3^{10}$	1.412(16)
Np1	$O2^3$	2.389(5)		C2	C3	1.412(16)
Np1	$O2^4$	2.389(5)		C2	$C3^9$	1.412(16)
Np1	$O1B^5$	2.407(10)		O1A	$Np1^8$	2.206(3)
Np1	$O1B^4$	2.407(10)		O1A	$Np1^7$	2.206(3)

Np1	O1B	2.407(10)		C5	C5[11]	1.42(4)
Np1	O1B[6]	2.407(10)		C5	C4[9]	1.379(18)
Np1	O1W	2.65(3)		C5	C4	1.379(18)
Np1	O1A[6]	2.206(3)		C5	C4[5]	1.379(18)
Np1	O1A[4]	2.206(3)		C5	C4[10]	1.379(18)
Np1	O1A[5]	2.206(3)		C3	C3[5]	0.87(3)
Np1	O1A	2.206(3)		C3	C4	1.43(2)
O2	C1	1.263(8)		C3	C4[5]	1.68(2)
O1B	Np1[7]	2.407(10)		C4	C3[5]	1.68(2)
O1B	Np1[8]	2.407(10)		C4	C4[5]	0.89(3)
C1	O2[9]	1.263(8)				

[1]1-Y,1-Z,1-X; [2]1-Z,+Y,1-X; [3]+Z,+Y,1-X; [4]+X,+Y,1-Z; [5]1-X,+Y,+Z; [6]1-X,+Y,1-Z; [7]+Y,+Z,+X; [8]+Z,+X,+Y; [9]1-X,+Z,+Y; [10]+X,+Z,+Y; [11]1-X,1/2-Y,1/2-Z

II.41 Np-NH_2-tpdc

Table 1 Crystal data and structure refinement for Np-NH2-tpdc.	
Identification code	Th-NH2-tpdc
Empirical formula	$C_{192}Np_{12}O_{76}$
Formula weight	6365.92
Temperature/K	100.0
Crystal system	cubic
Space group	Fm-3m
a/Å	33.3917(9)
b/Å	33.3917(9)
c/Å	33.3917(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	37232(3)
Z	2
ρ_{calc}g/cm^3	0.568
μ/mm^{-1}	1.682
F(000)	5752.0
Crystal size/mm^3	0.254 × 0.136 × 0.124
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.88 to 52.71
Index ranges	-41 ≤ h ≤ 27, -41 ≤ k ≤ 41, -33 ≤ l ≤ 41
Reflections collected	32772
Independent reflections	1929 [R_{int} = 0.0688, R_{sigma} = 0.0209]
Data/restraints/parameters	1929/11/30
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0643, wR_2 = 0.1864
Final R indexes [all data]	R_1 = 0.0840, wR_2 = 0.2113
Largest diff. peak/hole / e Å^{-3}	2.13/-2.19

Annexes

Table 2 Fractional Atomic Coordinates ($\times10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2\times10^3$) for Np-NH2-tpdc. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np1	5797.3(2)	5000	5000	42.2(3)
O2	5373(3)	5373(3)	4627(3)	86(6)
O1	6116(3)	5638(3)	5000	104(3)
C1	5984(4)	5984(4)	5000	114(8)
O3W	6654(19)	5000	5000	290(30)
C2	6304(4)	6304(4)	5000	100
C4	6463(4)	7017(4)	5000	100
C5	6870(5)	6870(5)	5000	100
C6	7190(5)	7190(5)	5000	100
C3	6169(4)	6709(4)	5000	100
C8	7322(8)	7322(8)	5377(9)	100
C7	7090(12)	7591(6)	5000	100

Table 3 Anisotropic Displacement Parameters ($Å^2\times10^3$) for Np-NH2-tpdc. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np1	19.2(4)	53.7(4)	53.7(4)	0	0	0
O2	86(6)	86(6)	86(6)	-44(6)	-44(6)	44(6)
O1	60(5)	103(8)	150(10)	0	0	-49(5)
O3W	420(80)	220(30)	220(30)	0	0	0

Table 4 Bond Lengths for Np-NH2-tpdc.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	Np1[1]	3.7650(8)		C1	O1[10]	1.236(13)
Np1	Np1[2]	3.7650(8)		C1	C2	1.511(16)
Np1	Np1[3]	3.7650(8)		C2	C3[10]	1.425(12)
Np1	O2[4]	2.261(5)		C2	C3	1.425(12)
Np1	O2	2.261(5)		C4	C5	1.446(12)
Np1	O2[5]	2.261(5)		C4	C3	1.421(14)
Np1	O2[6]	2.261(5)		C5	C4[10]	1.446(12)
Np1	O1[7]	2.382(9)		C5	C6	1.512(17)
Np1	O1[4]	2.382(9)		C6	C8	1.406(18)
Np1	O1	2.382(9)		C6	C8[6]	1.406(18)
Np1	O1[8]	2.382(9)		C6	C7[10]	1.380(18)
Np1	O3W	2.86(6)		C6	C7	1.380(18)
O2	Np1[9]	2.261(5)		C8	C8[11]	1.68(7)
O2	Np1[2]	2.261(5)		C7	C7[12]	1.51(7)
O1	C1	1.237(13)				

[1]+Y,+Z,+X; [2]1-Y,1-Z,1-X; [3]1-Z,1-X,1-Y; [4]+X,1-Y,+Z; [5]+X,1-Y,1-Z; [6]+X,+Y,1-Z; [7]+X,+Z,+Y; [8]+X,+Z,1-Y; [9]+Z,+X,+Y; [10]+Y,+X,1-Z; [11]3/2-X,3/2-Y,+Z; [12]3/2-Y,3/2-X,+Z

II.42 Np_{38}-THF

Table 1 Crystal data and structure refinement for Np38-THF.	
Identification code	Np38-THF
Empirical formula	C_{200} C_{l18} Np_{38} O_{112} H_{184}
Formula weight	14025.54
Temperature/K	293
Crystal system	tetragonal
Space group	I 4/m
a/Å	21.9347
b/Å	21.9347
c/Å	29.8559
α/°	90
β/°	90
γ/°	90
Volume/Å^3	14364.6
Z	2
ρ_{calc}g/cm^3	3.2374
μ/mm^{-1}	13.844
F(000)	12240
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.19 to 26.43
Index ranges	-27 ≤ h ≤ 27, -27 ≤ k ≤ 27, -37 ≤ l ≤ 37
Reflections collected	165896
Independent reflections	7543 [R_{int} = 0.0618, R_{sigma} = 0.0209]
Data/restraints/parameters	253/12/52
Goodness-of-fit on F^2	3.57
Final R indexes [I>=2σ (I)]	R_1 = 0.0674, wR_2 = 0.0841
Final R indexes [all data]	R_1 = 0.1151, wR_2 = 0.0857
Largest diff. peak/hole / e Å^{-3}	12.66/-4.24

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np38-THF. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Np1	0.5	0.5	0.59121(4)	0.0095(3)
Np2	0.62369(3)	0.49350(3)	0.5	0.0097(3)
Np3	0.61720(3)	0.36830(3)	0.59189(2)	0.01673(19)
Np4	0.73479(4)	0.36101(4)	0.5	0.0223(3)
Np5	0.61463(4)	0.25153(4)	0.5	0.0234(3)
Np6	0.48541(3)	0.25742(3)	0.59301(2)	0.0230(2)
Np7	0.49086(3)	0.37447(3)	0.67942(2)	0.0231(2)
Cl1	0.5	0.5	0.7196(3)	0.033(2)
Cl2	0.4842(2)	0.1988(2)	0.5	0.0277(19)
Cl3	0.80585(17)	0.37388(18)	0.57815(15)	0.0337(14)

Cl4	0.5680(12)	0.1707(12)	0.5845(9)	0.208(11)
O1f	0.5660(3)	0.5590(3)	0.5459(3)	0.008(3)
O2f	0.6831(4)	0.4288(4)	0.4540(3)	0.019(3)
O3f	0.4344(4)	0.4433(4)	0.6362(3)	0.017(3)
O4f	0.4308(4)	0.3230(4)	0.6332(3)	0.027(3)
O5f	0.6726(4)	0.3087(4)	0.4560(3)	0.025(3)
O6f	0.5518(4)	0.3101(4)	0.5463(3)	0.022(3)
O10f	0.5489(5)	0.3131(4)	0.6347(4)	0.033(4)
O9a	0.4805(4)	0.2768(4)	0.7139(3)	0.038(3)
O12a	0.4707(8)	0.2067(6)	0.6608(5)	0.043(3)
C1a	0.4423(8)	0.1792(7)	0.7341(6)	0.042(4)
C2a	0.4200(11)	0.1245(8)	0.7202(7)	0.097(7)
C3a	0.4667(8)	0.2244(6)	0.7027(6)	0.038(4)
C4a	0.4400(8)	0.1962(8)	0.7783(6)	0.063(6)
C7a	0.4168(10)	0.1538(9)	0.8091(7)	0.087(7)
C9a	0.3992(13)	0.0829(9)	0.7526(8)	0.147(12)
C11a	0.3985(12)	0.0978(10)	0.7957(8)	0.134(9)
H1c2a	0.4185	0.1145	0.6889	0.1164
H1c4a	0.4537	0.2357	0.7878	0.0754
H1c7a	0.414	0.1646	0.8402	0.104
H1c9a	0.3854	0.0433	0.7435	0.1772
H1c11a	0.3848	0.0686	0.8174	0.1602
O9b	0.710(2)	0.202(6)	0.5055(15)	0.038(3)
O12b	0.787(6)	0.266(2)	0.4956(14)	0.043(3)
C1b	0.8110(8)	0.1630(9)	0.5084(9)	0.042(4)
C2b	0.8713(16)	0.173(3)	0.5006(12)	0.097(8)
C3b	0.765(3)	0.211(3)	0.5038(12)	0.038(4)
C4b	0.789(3)	0.1060(15)	0.5186(11)	0.063(6)
C7b	0.832(6)	0.0589(17)	0.5232(15)	0.087(7)
C9b	0.9123(18)	0.125(5)	0.5071(16)	0.145(11)
C11b	0.893(5)	0.070(5)	0.5184(17)	0.132(10)
H1c2b	0.8855	0.2123	0.4909	0.1164
H1c4b	0.7465	0.0987	0.5225	0.0754
H1c7b	0.8183	0.0183	0.5298	0.104
H1c9b	0.9552	0.1314	0.5034	0.1772
H1c11b	0.9212	0.0373	0.5233	0.1602
O9c	0.5866(9)	0.3845(8)	0.7197(4)	0.038(3)
O12c	0.6220(11)	0.4611(8)	0.7607(6)	0.043(3)
C1c	0.6055(9)	0.3671(8)	0.7970(5)	0.042(4)
C2c	0.6310(12)	0.3878(11)	0.8357(6)	0.097(8)
C3c	0.6029(10)	0.4046(9)	0.7563(5)	0.038(4)
C4c	0.5835(10)	0.3088(9)	0.7934(6)	0.063(6)
C7c	0.5854(12)	0.2720(10)	0.8318(8)	0.087(7)
C9c	0.6298(15)	0.3497(13)	0.8735(7)	0.147(13)
C11c	0.6070(15)	0.2938(13)	0.8711(8)	0.132(10)
H1c2c	0.6495	0.4274	0.8371	0.1164
H1c4c	0.5675	0.2937	0.7656	0.0754
H1c7c	0.571	0.2307	0.8302	0.104

H1c9c	0.6456	0.3643	0.9015	0.1772
H1c11c	0.6059	0.2686	0.8974	0.1602
O9d	0.599(4)	0.1898(19)	0.5673(11)	0.038(3)
O12d	0.513(2)	0.144(4)	0.5891(10)	0.043(3)
C1d	0.5987(10)	0.0820(8)	0.5748(8)	0.042(4)
C2d	0.569(2)	0.0314(15)	0.5901(11)	0.097(8)
C3d	0.571(2)	0.143(2)	0.5760(9)	0.038(4)
C4d	0.6576(15)	0.079(2)	0.5595(9)	0.063(6)
C7d	0.686(2)	0.022(4)	0.5580(11)	0.087(7)
C9d	0.599(4)	-0.0253(19)	0.5863(14)	0.149(13)
C11d	0.655(3)	-0.029(3)	0.5703(14)	0.133(10)
H1c2d	0.5294	0.0344	0.6031	0.1164
H1c4d	0.679	0.1153	0.5503	0.0754
H1c7d	0.7271	0.0184	0.548	0.104
H1c9d	0.5779	-0.0617	0.5954	0.1772
H1c11d	0.6742	-0.0683	0.5675	0.1602
O1ta	0.6772(6)	0.3001(6)	0.6424(4)	0.065(4)
C1ta	0.7150(11)	0.3192(13)	0.6794(7)	0.143(12)
C2ta	0.7577(16)	0.2655(17)	0.6897(12)	0.30(3)
C3ta	0.7179(18)	0.2109(14)	0.6765(14)	0.54(5)
C4ta	0.6848(13)	0.2359(10)	0.6351(10)	0.31(3)
H1c1ta	0.7388	0.354	0.6707	0.1715
H2c1ta	0.6899	0.3273	0.705	0.1715
H1c2ta	0.7658	0.2641	0.7213	0.3616
H2c2ta	0.7927	0.2674	0.6704	0.3616
H1c3ta	0.7435	0.1774	0.6679	0.6458
H2c3ta	0.6888	0.203	0.6998	0.6458
H1c4ta	0.6455	0.2169	0.6326	0.3704
H2c4ta	0.7095	0.2294	0.609	0.3704

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) Np38-THF. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Np1	0.0075(4)	0.0075(4)	0.0135(7)	0	0	0
Np2	0.0047(4)	0.0087(4)	0.0157(5)	0.0006(3)	0	0
Np3	0.0149(3)	0.0131(3)	0.0222(4)	0.0031(2)	-0.0021(2)	0.0022(2)
Np4	0.0155(5)	0.0174(5)	0.0340(6)	0.0049(4)	0	0
Np5	0.0220(5)	0.0123(5)	0.0359(6)	0.0044(4)	0	0
Np6	0.0237(4)	0.0149(3)	0.0305(4)	-0.0017(3)	0.0004(3)	0.0053(3)
Np7	0.0226(4)	0.0210(4)	0.0257(4)	-0.0007(3)	0.0009(3)	0.0057(3)
Cl1	0.033(3)	0.033(3)	0.033(5)	0	0	0
Cl2	0.028(3)	0.017(3)	0.038(4)	-0.003(2)	0	0
Cl3	0.025(2)	0.030(2)	0.046(3)	0.0054(18)	-0.006(2)	0.003(2)
O1f	0.009(5)	0.005(5)	0.009(5)	0.005(4)	0.000(4)	0.004(4)
O2f	0.002(5)	0.017(5)	0.037(7)	0.004(4)	-0.004(4)	0.000(5)
O3f	0.019(6)	0.018(5)	0.013(5)	0.006(4)	0.000(4)	-0.002(4)

O4f	0.031(6)	0.012(5)	0.038(7)	-0.003(5)	-0.012(5)	0.000(5)
O5f	0.012(5)	0.018(6)	0.044(7)	0.003(4)	0.003(5)	0.003(5)
O6f	0.021(6)	0.006(5)	0.039(7)	-0.001(4)	-0.007(5)	-0.003(5)
O10f	0.040(7)	0.025(6)	0.034(7)	0.000(5)	0.012(6)	0.001(5)
O9a	0.046(5)	0.025(4)	0.043(5)	-0.001(4)	0.013(4)	0.006(3)
O12a	0.049(5)	0.046(5)	0.034(5)	-0.010(4)	0.000(4)	0.004(4)
C1a	0.047(8)	0.031(7)	0.047(8)	-0.012(6)	0.010(6)	0.013(6)
C2a	0.162(16)	0.060(10)	0.069(11)	-0.033(11)	0.043(11)	-0.001(9)
C3a	0.020(6)	0.040(7)	0.054(8)	0.003(5)	0.011(6)	0.024(6)
C4a	0.057(9)	0.080(11)	0.052(9)	-0.035(8)	0.006(7)	0.014(8)
C7a	0.109(13)	0.092(13)	0.059(11)	-0.042(11)	0.013(9)	0.018(9)
C9a	0.26(3)	0.064(13)	0.116(17)	-0.066(15)	0.092(18)	0.021(12)
C11a	0.24(2)	0.074(13)	0.087(14)	-0.062(15)	0.076(16)	0.016(11)
O9b	0.028(4)	0.035(5)	0.051(5)	0.008(4)	-0.009(4)	-0.006(4)
O12b	0.042(5)	0.036(5)	0.051(5)	0.005(4)	0.006(4)	0.007(4)
C1b	0.029(7)	0.041(8)	0.055(8)	0.018(6)	-0.001(6)	-0.002(6)
C2b	0.053(11)	0.052(13)	0.186(16)	0.011(9)	-0.008(10)	0.003(11)
C3b	0.045(7)	0.042(8)	0.026(7)	0.026(6)	-0.007(5)	-0.013(5)
C4b	0.062(11)	0.049(9)	0.077(9)	0.025(8)	0.029(7)	0.005(7)
C7b	0.075(13)	0.057(11)	0.128(13)	0.028(9)	0.022(10)	0.017(9)
C9b	0.054(14)	0.07(2)	0.31(2)	0.047(13)	-0.023(14)	-0.005(17)
C11b	0.061(15)	0.056(17)	0.28(2)	0.038(12)	-0.011(14)	0.007(15)
O9c	0.055(5)	0.036(5)	0.022(4)	0.007(4)	0.001(4)	0.004(3)
O12c	0.047(5)	0.040(5)	0.042(5)	-0.007(4)	-0.006(4)	0.008(4)
C1c	0.055(8)	0.047(8)	0.023(7)	0.005(6)	-0.005(6)	0.013(6)
C2c	0.181(16)	0.058(13)	0.052(11)	-0.012(11)	-0.022(11)	0.012(9)
C3c	0.033(7)	0.049(8)	0.031(7)	0.021(5)	0.007(5)	0.020(6)
C4c	0.063(9)	0.062(9)	0.064(11)	-0.005(7)	-0.027(8)	0.031(8)
C7c	0.113(13)	0.074(12)	0.073(13)	-0.019(9)	-0.027(10)	0.036(9)
C9c	0.31(3)	0.09(2)	0.040(13)	-0.006(17)	-0.039(14)	0.039(12)
C11c	0.27(2)	0.074(17)	0.051(14)	-0.018(15)	-0.038(14)	0.039(12)
O9d	0.037(5)	0.022(5)	0.054(5)	0.002(3)	-0.008(4)	-0.002(4)
O12d	0.042(5)	0.038(5)	0.048(5)	0.007(4)	0.009(4)	0.004(4)
C1d	0.051(8)	0.019(7)	0.055(8)	0.009(6)	-0.003(6)	0.003(6)
C2d	0.061(13)	0.045(12)	0.184(16)	0.009(9)	0.013(11)	0.009(10)
C3d	0.056(8)	0.026(8)	0.031(7)	0.018(6)	-0.020(5)	-0.004(5)
C4d	0.071(10)	0.050(11)	0.067(9)	0.028(7)	0.012(7)	0.025(7)
C7d	0.084(12)	0.058(13)	0.118(13)	0.032(9)	0.025(9)	0.020(10)
C9d	0.102(19)	0.025(15)	0.32(3)	0.027(12)	0.009(16)	0.015(14)
C11d	0.085(17)	0.035(15)	0.28(2)	0.031(12)	0.022(15)	0.016(14)

Table 4 Bond Lengths for Np38-THF.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np1	O1f	2.367(7)		C9b	C11b^iv^	1.49(13)
Np1	O1f^i^	2.367(7)		C9b	H1c2b	2.06(10)

Np1	O1f^ii^	2.367(7)		C9b	H1c2b^iv^	2.00(11)
Np1	O1f^iii^	2.367(7)		C9b	H1c9b	0.96(4)
Np1	O3f	2.328(9)		C9b	H1c9b^iv^	1.00(4)
Np1	O3f^i^	2.328(9)		C9b	H1c11b	1.99(11)
Np1	O3f^ii^	2.328(9)		C9b	H1c11b^iv^	2.14(10)
Np1	O3f^iii^	2.328(9)		C11b	C11b^iv^	1.10(7)
Np2	O1f	2.354(7)		C11b	H1c7b	2.02(11)
Np2	O1f^iii^	2.365(7)		C11b	H1c7b^iv^	2.46(9)
Np2	O1f^iv^	2.354(7)		C11b	H1c9b	1.97(11)
Np2	O1f^v^	2.365(7)		C11b	H1c9b^iv^	2.03(11)
Np2	O2f	2.366(9)		C11b	H1c11b	0.96(11)
Np2	O2f^iv^	2.366(9)		C11b	H1c11b^iv^	1.56(8)
Np2	O6f^ii^	2.378(9)		H1c2b	H1c2b^iv^	0.546
Np2	O6f^vi^	2.378(9)		H1c2b	H1c9b	2.3721
Np3	O1f^iii^	2.365(7)		H1c2b	H1c9b^iv^	2.3487
Np3	O2f^iv^	2.393(9)		H1c4b	H1c4b^iv^	1.3417
Np3	O3f^ii^	2.369(9)		H1c4b	H1c7b	2.3734
Np3	O4f^ii^	2.263(9)		H1c4b	C4d	2.28(3)
Np3	O5f^iv^	2.287(9)		H1c4b	C7d	2.39(7)
Np3	O6f	2.354(9)		H1c4b	H1c4d	1.7372
Np3	O10f	2.312(11)		H1c4b	H1c7d	1.9653
Np3	O1ta	2.499(13)		H1c7b	H1c7b^iv^	1.7779
Np4	O2f	2.320(9)		H1c7b	H1c9b^vii^	1.9369
Np4	O2f^iv^	2.320(9)		H1c7b	H1c9b^viii^	2.0278
Np4	O5f	2.214(9)		H1c7b	H1c11b	2.3034
Np4	O5f^iv^	2.214(9)		H1c7b	H1c7d	2.0735
Np4	O12b	2.38(7)		H1c9b	H1c9b^iv^	0.2026
Np4	O12b^iv^	2.38(7)		H1c9b	H1c11b	2.2753
Np5	O5f	2.217(9)		H1c9b	H1c11b^ix^	2.2186
Np5	O5f^iv^	2.217(9)		H1c9b	H1c11b^iv^	2.3364
Np5	O6f	2.337(9)		H1c9b	H1c11b^x^	2.2812
Np5	O6f^iv^	2.337(9)		H1c11b	H1c11b^iv^	1.3894
Np5	O9b	2.36(7)		O9c	O12c	2.22(2)
Np5	O9b^iv^	2.36(7)		O9c	C1c	2.38(2)
Np5	O9d	2.45(4)		O9c	C3c	1.23(2)
Np5	O9d^iv^	2.45(4)		O9c	H1c4c	2.454(16)
Np6	O2f^v^	2.283(9)		O12c	C1c	2.36(2)
Np6	O4f	2.223(9)		O12c	C3c	1.31(3)
Np6	O6f	2.324(9)		O12c	H1c2c	2.471(18)
Np6	O10f	2.232(11)		C1c	C2c	1.36(3)
Np6	O12a	2.332(15)		C1c	C3c	1.47(2)
Np7	O3f	2.341(9)		C1c	C4c	1.37(3)
Np7	O3f^ii^	2.341(9)		C1c	C7c	2.37(3)
Np7	O4f	2.217(9)		C1c	C9c	2.38(3)
Np7	O10f	2.284(11)		C1c	H1c2c	2.028(17)
Np7	O9a	2.388(9)		C1c	H1c4c	2.041(17)
Np7	O9c	2.430(18)		C2c	C3c	2.48(2)
Cl4	O9d	0.95(7)		C2c	C4c	2.38(3)

Cl4	O12d	1.35(6)		C2c	C9c	1.40(3)
Cl4	C1d	2.08(3)		C2c	C11c	2.38(4)
Cl4	C3d	0.66(5)		C2c	H1c2c	0.96(2)
Cl4	H1c4ta	2.44(3)		C2c	H1c9c	2.056(19)
O4f	H1c1ta^iii^	2.435(9)		C3c	C4c	2.41(3)
O9a	O12a	2.219(17)		C4c	C7c	1.40(3)
O9a	C1a	2.377(18)		C4c	C11c	2.40(3)
O9a	C3a	1.235(16)		C4c	H1c4c	0.960(19)
O9a	H1c4a	2.456(9)		C4c	H1c7c	2.053(19)
O9a	H1c4c	2.482(9)		C7c	C9c	2.32(4)
O12a	C1a	2.35(2)		C7c	C11c	1.35(4)
O12a	C3a	1.31(2)		C7c	H1c4c	2.07(2)
O12a	H1c2a	2.471(14)		C7c	H1c7c	0.96(2)
C1a	C2a	1.36(2)		C7c	H1c11c	2.01(2)
C1a	C3a	1.47(2)		C9c	C11c	1.33(4)
C1a	C4a	1.37(3)		C9c	H1c2c	2.07(3)
C1a	C7a	2.37(3)		C9c	H1c9c	0.96(2)
C1a	C9a	2.38(3)		C9c	H1c11c	1.99(3)
C1a	H1c2a	2.028(17)		C11c	H1c7c	2.01(3)
C1a	H1c4a	2.042(17)		C11c	H1c9c	1.98(3)
C2a	C3a	2.47(2)		C11c	H1c11c	0.96(3)
C2a	C4a	2.38(3)		H1c2c	H1c9c	2.3721
C2a	C9a	1.41(3)		H1c4c	H1c7c	2.3735
C2a	C11a	2.38(3)		H1c7c	H1c11c	2.3034
C2a	H1c2a	0.96(2)		H1c9c	H1c11c	2.2753
C2a	H1c9a	2.057(19)		H1c11c	H1c11d^xi^	2.4633
C3a	C4a	2.41(3)		O9d	O12d	2.23(9)
C4a	C7a	1.40(3)		O9d	C1d	2.38(5)
C4a	C11a	2.40(3)		O9d	C3d	1.22(7)
C4a	H1c4a	0.960(18)		O9d	H1c4d	2.45(7)
C4a	H1c7a	2.054(18)		O9d	H1c4ta	2.28(5)
C7a	C9a	2.33(3)		O12d	C1d	2.36(7)
C7a	C11a	1.35(3)		O12d	C3d	1.33(6)
C7a	H1c4a	2.07(2)		O12d	H1c2d	2.47(9)
C7a	H1c7a	0.96(2)		C1d	C2d	1.37(4)
C7a	H1c11a	2.01(2)		C1d	C3d	1.47(5)
C9a	C11a	1.33(3)		C1d	C4d	1.37(4)
C9a	H1c2a	2.07(2)		C1d	C7d	2.38(6)
C9a	H1c9a	0.96(2)		C1d	C9d	2.38(5)
C9a	H1c11a	1.99(2)		C1d	H1c2d	2.03(2)
C11a	H1c7a	2.01(2)		C1d	H1c4d	2.04(2)
C11a	H1c9a	1.98(2)		C2d	C3d	2.48(5)
C11a	H1c11a	0.96(2)		C2d	C4d	2.39(5)
H1c2a	H1c9a	2.3721		C2d	C9d	1.41(7)
H1c4a	H1c7a	2.3735		C2d	C11d	2.38(8)
H1c7a	H1c11a	2.3034		C2d	H1c2d	0.95(4)
H1c9a	H1c11a	2.2753		C2d	H1c9d	2.06(3)
O9b	O9b^iv^	0.33(6)		C3d	C4d	2.41(6)

O9b	O12b	2.22(14)		C4d	C7d	1.40(9)
O9b	O12b^iv^	2.20(14)		C4d	C11d	2.39(8)
O9b	C1b	2.38(7)		C4d	H1c4d	0.96(4)
O9b	C1b^iv^	2.41(6)		C4d	H1c7d	2.05(4)
O9b	C3b	1.22(8)		C7d	C9d	2.33(9)
O9b	C3b^iv^	1.25(8)		C7d	C11d	1.36(10)
O9b	H1c4b	2.46(12)		C7d	H1c4d	2.07(9)
O9b	H1c4d	2.42(11)		C7d	H1c7d	0.95(4)
O12b	O12b^iv^	0.26(6)		C7d	H1c11d	2.02(9)
O12b	C1b	2.35(6)		C9d	C11d	1.32(10)
O12b	C1b^iv^	2.32(6)		C9d	H1c2d	2.07(7)
O12b	C3b	1.32(9)		C9d	H1c9d	0.96(6)
O12b	C3b^iv^	1.30(9)		C9d	H1c11d	1.98(8)
O12b	H1c2b	2.46(12)		C11d	H1c7d	2.01(6)
O12b	H1c2b^iv^	2.49(12)		C11d	H1c9d	1.98(6)
C1b	C1b^iv^	0.50(4)		C11d	H1c11d	0.96(7)
C1b	C2b	1.36(4)		H1c2d	H1c2d^xii^	1.9861
C1b	C2b^iv^	1.37(4)		H1c2d	H1c9d	2.3721
C1b	C3b	1.46(7)		H1c2d	H1c9d^xii^	2.4383
C1b	C3b^iv^	1.50(7)		H1c4d	H1c7d	2.3734
C1b	C4b	1.37(4)		H1c7d	H1c11d	2.3034
C1b	C4b^iv^	1.56(4)		H1c9d	H1c11d	2.2753
C1b	C7b	2.37(5)		O1ta	C1ta	1.44(3)
C1b	C9b	2.37(6)		O1ta	C2ta	2.38(4)
C1b	C9b^iv^	2.42(6)		O1ta	C3ta	2.38(4)
C1b	H1c2b	2.029(19)		O1ta	C4ta	1.43(3)
C1b	H1c2b^iv^	1.960(18)		O1ta	H1c1ta	1.983(13)
C1b	H1c4b	2.041(19)		O1ta	H2c1ta	1.983(12)
C1b	H1c4b^iv^	2.20(2)		O1ta	H1c4ta	1.975(13)
C2b	C2b^iv^	0.04(5)		O1ta	H2c4ta	1.975(13)
C2b	C3b	2.48(8)		C1ta	C2ta	1.54(5)
C2b	C3b^iv^	2.48(8)		C1ta	C3ta	2.38(4)
C2b	C4b	2.39(7)		C1ta	C4ta	2.35(4)
C2b	C4b^iv^	2.40(7)		C1ta	H1c1ta	0.96(3)
C2b	C9b	1.40(10)		C1ta	H2c1ta	0.96(2)
C2b	C9b^iv^	1.40(10)		C1ta	H1c2ta	2.07(2)
C2b	C11b	2.37(12)		C1ta	H2c2ta	2.07(3)
C2b	C11b^iv^	2.38(12)		C2ta	C3ta	1.53(5)
C2b	H1c2b	0.96(6)		C2ta	C4ta	2.37(5)
C2b	H1c2b^iv^	0.95(6)		C2ta	H1c1ta	2.06(4)
C2b	H1c9b	2.06(4)		C2ta	H2c1ta	2.06(4)
C2b	H1c9b^iv^	2.06(4)		C2ta	H1c2ta	0.96(4)
C3b	C3b^iv^	0.23(5)		C2ta	H2c2ta	0.96(4)
C3b	C4b	2.40(7)		C2ta	H1c3ta	2.06(4)
C3b	C4b^iv^	2.46(7)		C2ta	H2c3ta	2.06(4)
C4b	C4b^iv^	1.11(5)		C3ta	C4ta	1.53(5)
C4b	C7b	1.41(11)		C3ta	H1c2ta	2.06(4)
C4b	C7b^iv^	1.87(9)		C3ta	H2c2ta	2.06(4)

C4b	C11b	2.41(13)		C3ta	H1c3ta	0.96(3)
C4b	H1c4b	0.95(6)		C3ta	H2c3ta	0.96(4)
C4b	H1c4b^iv^	1.55(5)		C3ta	H1c4ta	2.06(4)
C4b	H1c7b	2.05(4)		C3ta	H2c4ta	2.06(4)
C4b	H1c7b^iv^	2.49(4)		C4ta	H1c3ta	2.06(3)
C7b	C7b^iv^	1.39(6)		C4ta	H2c3ta	2.06(3)
C7b	C9b	2.33(13)		C4ta	H1c4ta	0.96(3)
C7b	C9b^iv^	2.45(12)		C4ta	H2c4ta	0.96(3)
C7b	C11b	1.37(17)		H1c1ta	H2c1ta	1.5952
C7b	C11b^iv^	1.84(13)		H1c1ta	H2c2ta	2.2369
C7b	H1c4b	2.07(12)		H2c1ta	H1c2ta	2.22
C7b	H1c4b^iv^	2.48(10)		H1c2ta	H1c2ta^xiii^	1.9472
C7b	H1c7b	0.96(5)		H1c2ta	H2c2ta	1.632
C7b	H1c7b^iv^	1.84(5)		H1c2ta	H2c3ta	2.2499
C7b	H1c9b^vii^	2.48(6)		H2c2ta	H1c3ta	2.2498
C7b	H1c11b	2.01(13)		H1c3ta	H2c3ta	1.6321
C7b	H1c11b^iv^	2.44(11)		H1c3ta	H2c4ta	2.2231
C9b	C9b^iv^	0.42(7)		H2c3ta	H1c4ta	2.2407
C9b	C11b	1.32(15)		H1c4ta	H2c4ta	1.5953

(i) -x+1,-y+1,z ; (ii) -y+1,x,z ; (iii) y,-x+1,z ; (iv) x,y,-z+1 ; (v) y,-x+1,-z+1 ; (vi) -y+1,x,-z+1 ; (vii) -y+1,x-1,z ; (viii) -y+1,x-1,-z+1 ; (ix) y+1,-x+1,z ; (x) y+1,-x+1,-z+1 ; (xi) -y+1/2,x-1/2,-z+3/2 ; (xii)-x+1,-y,z ; (xiii) -x+3/2,-y+1/2,-z+3/2

II.43 U_{38}-iPrOH

Table 1 Crystal data and structure refinement for U38-iPrOH.	
Identification code	U38-iPrOH
Empirical formula	$C_{60}H_{152}Cl_{42}O_{76}U_{38}$
Formula weight	12623.85
Temperature/K	299.43
Crystal system	tetragonal
Space group	I4/m
a/Å	19.6962(7)
b/Å	19.6962(7)
c/Å	29.9535(13)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	11620.2(10)
Z	2
ρ_{calc}g/cm^3	3.608
μ/mm^{-1}	26.904
F(000)	10660.0
Crystal size/mm^3	0.133 × 0.11 × 0.083

Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	2.474 to 56.54
Index ranges	-22 ≤ h ≤ 26, -24 ≤ k ≤ 23, -38 ≤ l ≤ 39
Reflections collected	47636
Independent reflections	7308 [R_{int} = 0.0657, R_{sigma} = 0.0772]
Data/restraints/parameters	7308/6/266
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0424, wR_2 = 0.0976
Final R indexes [all data]	R_1 = 0.1200, wR_2 = 0.1193
Largest diff. peak/hole / e $Å^{-3}$	3.19/-2.54

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for U38-iPrOH. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U7	5000	5000	5919.5(3)	15.3(2)
U6	4601.6(3)	6322.8(3)	5000	14.94(15)
U4	5947.8(2)	6743.9(2)	5928.1(2)	19.14(13)
U5	6370.5(2)	5401.6(2)	6795.9(2)	23.23(13)
U1	7202.0(3)	7148.6(3)	5000	23.14(17)
U2	7592.6(2)	5772.5(2)	5933.9(2)	22.86(13)
U3	5586.4(3)	7995.7(3)	5000	22.92(17)
Cl1	8028.6(17)	7116.8(17)	5781.6(11)	40.6(8)
O4	6380(4)	7541(4)	5430(2)	24.0(18)
O1	6793(4)	6255(3)	5455(2)	19.9(18)
O5	7154(4)	4959(4)	6347(2)	23.9(19)
O2	6775(4)	6206(4)	6345(2)	22.1(18)
O1SA	8319(4)	5992(5)	6574(3)	45(3)
C2SC	6178(12)	9742(9)	5000	53(6)
Cl7	5000	5000	7217.8(19)	34.7(15)
Cl4	5121.9(18)	8701.2(16)	5775.0(12)	40.4(8)
Cl6	6490.3(18)	4176.9(18)	7283.1(11)	45.4(9)
Cl5	7416.1(18)	5666(2)	7359.0(11)	50.4(10)
Cl3	7720(3)	8418(3)	5000	55.3(15)
O6	4134(3)	5464(3)	5461(2)	15.9(17)
O3	5463(4)	5844(4)	6367(2)	25.4(19)
O1AA	5071(3)	7186(4)	4549(2)	18.4(17)
O1SB	6397(6)	7663(5)	6387(4)	75(4)
C2SA	9043(8)	6193(10)	6637(6)	73(6)
C4SA	9041(10)	6842(10)	6885(8)	110(8)
C3SA	9408(10)	5656(12)	6882(9)	139(11)
O1SC	6300(5)	8989(6)	5000	37(3)

Cl2	8199(2)	5952(2)	5000	32.1(11)
C3SC	6463(11)	10018(9)	4576(7)	107(8)
C3	7110(30)	7710(30)	7020(20)	110(20)
C2	6480(40)	8030(30)	6720(20)	120(20)
C4	6260(30)	8680(20)	6782(17)	95(18)
C1	6720(20)	8800(20)	6542(15)	103(16)
C5	6874(18)	8110(16)	6509(11)	59(10)
C6	7340(20)	7870(30)	6848(17)	102(15)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U38-iPrOH. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U7	16.7(3)	16.7(3)	12.6(4)	0	0	0
U6	16.4(3)	14.0(3)	14.5(3)	0	0	0.4(3)
U4	20.5(3)	18.6(2)	18.3(2)	-1.86(18)	-1.02(18)	-1.07(19)
U5	25.7(3)	27.3(3)	16.7(2)	-1.2(2)	-3.96(19)	-1.1(2)
U1	20.8(4)	22.2(4)	26.4(4)	0	0	-5.5(3)
U2	19.1(3)	25.9(3)	23.6(3)	-1.3(2)	-3.9(2)	-2.3(2)
U3	25.8(4)	16.0(3)	27.0(4)	0	0	-1.8(3)
Cl1	44(2)	36(2)	42.1(19)	-1.5(16)	-12.9(16)	-12.8(17)
O4	25(4)	19(4)	28(5)	0(4)	0(4)	-4(4)
O1	21(4)	17(4)	22(4)	0(3)	-1(3)	-2(3)
O5	29(5)	26(5)	17(4)	1(4)	-3(4)	-5(4)
O2	24(4)	22(4)	21(4)	-1(3)	-2(3)	-3(3)
O1SA	38(6)	65(7)	32(6)	-2(5)	-14(4)	-12(5)
C2SC	73(17)	32(12)	55(14)	0	0	5(11)
Cl7	42(2)	42(2)	20(3)	0	0	0
Cl4	49(2)	28.4(19)	43.9(19)	-12.7(15)	5.0(17)	-7.9(16)
Cl6	52(2)	47(2)	38(2)	10.4(16)	-17.5(17)	-6.2(18)
Cl5	44(2)	73(3)	34.0(19)	-4.5(18)	-18.9(17)	-9(2)
Cl3	49(3)	32(3)	85(4)	0	0	-12(2)
O6	17(4)	16(4)	15(4)	0(3)	-3(3)	-3(3)
O3	24(5)	31(5)	21(4)	1(4)	-3(4)	4(4)
O1AA	17(4)	23(4)	16(4)	5(3)	2(3)	-3(3)
O1SB	108(10)	33(6)	85(9)	-29(6)	-38(7)	-17(6)
C2SA	51(11)	99(15)	68(12)	-33(11)	-6(9)	-23(11)
C4SA	90(17)	104(18)	140(20)	-23(15)	-47(15)	-14(13)
C3SA	76(16)	130(20)	210(30)	0(20)	-85(18)	43(15)
O1SC	23(7)	22(7)	66(9)	0	0	-5(5)
Cl2	20(2)	40(3)	36(3)	0	0	-6(2)
C3SC	170(20)	45(12)	105(17)	25(11)	17(16)	-25(13)

Table 4 Bond Lengths for U38-iPrOH.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U7	U5[1]	3.8474(7)		U1	O4[6]	2.209(7)
U7	U5[2]	3.8474(7)		U1	O4	2.209(7)
U7	U5	3.8474(7)		U1	O1[6]	2.367(7)
U7	U5[3]	3.8474(7)		U1	O1	2.367(7)
U7	O6	2.374(6)		U1	Cl3	2.701(5)
U7	O6[3]	2.374(6)		U1	Cl2	3.068(5)
U7	O6[1]	2.374(6)		U2	U6[4]	3.8240(6)
U7	O6[2]	2.374(6)		U2	U4[1]	3.7781(6)
U7	O3[1]	2.323(7)		U2	Cl1	2.821(3)
U7	O3	2.323(7)		U2	O1	2.333(7)
U7	O3[3]	2.323(7)		U2	O5	2.200(7)
U7	O3[2]	2.323(7)		U2	O2	2.199(7)
U6	U6[4]	3.8481(8)		U2	O1SA	2.431(8)
U6	U2[3]	3.8241(6)		U2	Cl4[1]	2.846(3)
U6	U2[5]	3.8241(6)		U2	O1AA[4]	2.344(7)
U6	U3	3.8235(8)		U2	Cl2	3.0621(17)
U6	O1[3]	2.358(7)		U3	U4[6]	3.7833(6)
U6	O1[5]	2.358(7)		U3	O4[6]	2.214(7)
U6	O6[4]	2.366(7)		U3	O4	2.214(7)
U6	O6	2.369(7)		U3	Cl4[6]	2.856(3)
U6	O6[6]	2.369(7)		U3	Cl4	2.856(3)
U6	O6[1]	2.366(7)		U3	O1AA	2.322(7)
U6	O1AA	2.360(7)		U3	O1AA[6]	2.322(7)
U6	O1AA[6]	2.360(7)		U3	O1SC	2.408(11)
U4	U5[3]	3.7897(6)		U3	Cl2[3]	3.056(4)
U4	U2	3.7625(6)		O1	U6[4]	2.358(7)
U4	U2[3]	3.7781(6)		O5	U4[1]	2.327(7)
U4	U3	3.7833(6)		O1SA	C2SA	1.491(16)
U4	O4	2.326(7)		C2SC	O1SC	1.503(19)
U4	O1	2.389(7)		C2SC	C3SC	1.49(2)
U4	O5[3]	2.327(7)		C2SC	C3SC[6]	1.49(2)
U4	O2	2.311(7)		Cl7	U5[1]	3.084(2)
U4	O6[1]	2.420(7)		Cl7	U5[3]	3.084(2)
U4	O3	2.405(7)		Cl7	U5[2]	3.084(2)
U4	O1AA[6]	2.406(7)		Cl4	U2[3]	2.846(3)
U4	O1SB	2.439(9)		Cl6	U5[1]	2.809(3)
U5	U4[1]	3.7897(6)		O6	U6[3]	2.366(6)
U5	U2	3.6047(6)		O6	U4[3]	2.420(7)
U5	O5	2.226(7)		O3	U5[3]	2.371(7)
U5	O2	2.229(7)		O1AA	U4[6]	2.405(7)

U5	Cl7	3.084(2)		O1AA	U2[5]	2.344(7)
U5	Cl6[3]	2.809(3)		O1SB	C2	1.25(6)
U5	Cl6	2.829(3)		O1SB	C5	1.34(3)
U5	Cl5	2.712(3)		C2SA	C4SA	1.48(2)
U5	O3[1]	2.371(7)		C2SA	C3SA	1.47(2)
U5	O3	2.367(7)		Cl2	U2[6]	3.0622(17)
U1	U6[4]	3.8579(8)		Cl2	U3[4]	3.056(4)
U1	U4[6]	3.8036(6)		C3	C2	1.66(7)
U1	U3	3.5930(9)		C2	C4	1.37(6)
U1	Cl1	2.852(3)		C1	C5	1.40(4)
U1	Cl1[6]	2.852(3)		C5	C6	1.44(5)

[1]+Y,1-X,+Z; [2]1-X,1-Y,+Z; [3]1-Y,+X,+Z; [4]+Y,1-X,1-Z; [5]1-Y,+X,1-Z; [6]+X,+Y,1-Z

Table 5 Atomic Occupancy for U38-iPrOH.

Atom	***Occupancy***		**Atom**	***Occupancy***		**Atom**	***Occupancy***
C3	0.45(4)		H3A	0.45(4)		H3B	0.45(4)
H3C	0.45(4)		C2	0.45(4)		H2	0.45(4)
C4	0.45(4)		H4A	0.45(4)		H4B	0.45(4)
H4C	0.45(4)		C1	0.55(4)		H1A	0.55(4)
H1B	0.55(4)		H1C	0.55(4)		C5	0.55(4)
H5	0.55(4)		C6	0.55(4)		H6A	0.55(4)
H6B	0.55(4)		H6C	0.55(4)			

II.44 Np$_{38}$-iPrOH

Table 1 Crystal data and structure refinement for Np38-iPrOH.

Identification code	Np38-iPrOH
Empirical formula	$C_{60}Cl_{42}$Np38-iPrOHO_{76}
Formula weight	12431.50
Temperature/K	99.99
Crystal system	tetragonal
Space group	I4/m
a/Å	19.5620(8)
b/Å	19.5620(8)
c/Å	29.3799(15)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	11242.9(11)
Z	2

ρ_{calc}g/cm^3	3.672
μ/mm^{-1}	17.936
F(000)	10432.0
Crystal size/mm^3	0.067 × 0.042 × 0.041
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.652 to 52.742
Index ranges	-24 ≤ h ≤ 20, -20 ≤ k ≤ 24, -25 ≤ l ≤ 36
Reflections collected	25716
Independent reflections	5873 [R_{int} = 0.0711, R_{sigma} = 0.0742]
Data/restraints/parameters	5873/0/195
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0536, wR_2 = 0.1065
Final R indexes [all data]	R_1 = 0.1116, wR_2 = 0.1226
Largest diff. peak/hole / e Å^{-3}	1.90/-4.39

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for Np38-iPrOH. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Np7	5000	5000	4071.7(4)	7.4(3)
Np6	6314.7(4)	5414.7(4)	5000	6.9(2)
Np4	5924.3(3)	6756.3(3)	4062.5(2)	8.85(16)
Np2	7579.0(3)	5806.9(3)	4061.4(2)	10.33(17)
Np3	7997.4(4)	4458.1(4)	5000	10.5(2)
Np5	6360.7(3)	5422.8(3)	3191.1(2)	10.97(16)
Np1	7169.0(4)	7170.4(4)	5000	10.6(2)
Cl2	8181(3)	6001(3)	5000	13.4(12)
Cl7	5000	5000	2754(3)	17.8(18)
Cl1	7994(2)	7164(2)	5798.1(14)	17.8(9)
Cl4	8715(2)	4928(2)	4222.8(15)	19.6(10)
Cl6	5807(2)	6514(2)	2692.6(14)	20.1(10)
Cl5	7395(2)	5699(2)	2610.4(14)	23.4(10)
Cl3	7687(3)	8456(3)	5000	25.6(15)
O2	6768(5)	6242(5)	3641(3)	9(2)
O4	6344(5)	7558(5)	5437(3)	12(2)
O1SA	6303(7)	7683(7)	3576(5)	39(4)
O7	7191(5)	4957(5)	4544(3)	8(2)
O1	6776(5)	6286(5)	4547(4)	17(3)
O3	5455(5)	5861(5)	3609(4)	17(3)
O6	5454(5)	5866(5)	5467(3)	12(2)
O1SC	8979(7)	3745(7)	5000	15(4)
O1SB	8284(5)	6037(5)	3419(4)	18(3)
C3SA	7277(12)	7760(12)	3064(8)	57(7)

C4SA	6549(13)	8795(14)	3368(9)	66(8)
C2SA	6848(14)	8110(14)	3479(10)	77(8)
O5	7145(5)	4981(5)	3638(3)	14(3)
C2SB	9013(10)	6236(10)	3350(6)	31(5)
C4SB	9370(12)	5653(12)	3106(8)	57(7)
C3SB	9039(11)	6911(11)	3094(8)	49(6)
C2SC	9731(12)	3882(12)	5000	20(6)
C3SC	10028(10)	3545(10)	4573(7)	39(5)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for Np38-iPrOH. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Np7	8.5(4)	8.5(4)	5.2(7)	0	0	0
Np6	7.0(5)	7.6(5)	6.0(4)	0	0	0.0(4)
Np4	10.5(3)	9.0(3)	7.1(4)	2.0(2)	1.1(3)	0.0(3)
Np2	8.1(3)	12.0(3)	10.9(4)	1.3(3)	2.9(3)	-1.2(3)
Np3	5.8(5)	11.5(5)	14.1(5)	0	0	0.7(4)
Np5	12.5(3)	13.6(3)	6.8(3)	0.6(3)	3.3(3)	-0.7(3)
Np1	8.6(5)	8.5(5)	14.6(5)	0	0	-2.1(4)
Cl2	9(3)	17(3)	15(3)	0	0	-4(2)
Cl7	22(3)	22(3)	9(4)	0	0	0
Cl1	23(2)	13(2)	17(2)	-3.0(17)	-5.8(18)	-1.3(19)
Cl4	14(2)	24(2)	21(2)	3.3(19)	6.4(18)	4.1(19)
Cl6	23(2)	25(2)	12(2)	9.9(18)	5.4(18)	0(2)
Cl5	24(2)	33(3)	13(2)	-1.9(19)	7.9(18)	-4(2)
Cl3	21(3)	18(3)	38(4)	0	0	2(3)
O2	18(6)	5(5)	6(6)	-3(4)	1(5)	-5(5)
O7	11(5)	11(5)	2(6)	2(4)	3(4)	-1(5)
O1	22(6)	18(6)	10(7)	-1(5)	9(5)	-1(5)
O3	24(7)	10(6)	17(6)	6(5)	2(5)	9(5)
O5	17(6)	18(6)	6(6)	-4(5)	4(5)	-3(5)

Table 4 Bond Lengths for Np38-iPrOH.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Np7	Np5	3.8029(10)		Np3	Cl4	2.834(4)
Np7	$Np5^1$	3.8030(10)		Np3	$Cl4^4$	2.834(4)
Np7	$Np5^2$	3.8030(10)		Np3	$O4^5$	2.202(10)
Np7	$Np5^3$	3.8030(10)		Np3	$O4^1$	2.202(10)
Np7	O3	2.339(10)		Np3	O7	2.288(10)
Np7	$O3^2$	2.339(10)		Np3	$O7^4$	2.288(10)
Np7	$O3^3$	2.339(10)		Np3	O1SC	2.373(14)

Np7	O3^{1}	2.339(10)		Np5	Np4^{1}	3.7548(9)
Np7	O6^{4}	2.346(10)		Np5	Cl7	3.069(3)
Np7	O6^{5}	2.346(10)		Np5	Cl6	2.806(4)
Np7	O6^{6}	2.346(10)		Np5	Cl6^{1}	2.833(4)
Np7	O6^{7}	2.346(10)		Np5	Cl5	2.702(4)
Np6	Np6^{5}	3.8138(12)		Np5	O2	2.225(9)
Np6	Np2	3.7827(8)		Np5	O3	2.320(10)
Np6	Np2^{4}	3.7826(8)		Np5	O3^{1}	2.326(10)
Np6	Np3	3.7865(12)		Np5	O5	2.196(10)
Np6	O7^{4}	2.353(10)		Np1	Np4^{4}	3.7644(9)
Np6	O7	2.353(10)		Np1	Np3^{2}	3.5705(13)
Np6	O1	2.344(10)		Np1	Cl2	3.025(6)
Np6	O1^{4}	2.344(10)		Np1	Cl1	2.847(4)
Np6	O6	2.344(10)		Np1	Cl1^{4}	2.847(4)
Np6	O6^{5}	2.353(10)		Np1	Cl3	2.712(6)
Np6	O6^{1}	2.353(10)		Np1	O4	2.196(10)
Np6	O6^{4}	2.344(10)		Np1	O4^{4}	2.196(10)
Np4	Np2	3.7319(9)		Np1	O1	2.314(11)
Np4	Np2^{2}	3.7495(9)		Np1	O1^{4}	2.314(11)
Np4	Np3^{2}	3.7470(9)		Cl2	Np2^{4}	3.022(2)
Np4	Np5	3.7536(9)		Cl7	Np5^{2}	3.069(3)
Np4	O2	2.296(10)		Cl7	Np5^{3}	3.069(3)
Np4	O4^{4}	2.303(10)		Cl7	Np5^{1}	3.069(3)
Np4	O1SA	2.425(13)		Cl1	Np2^{4}	2.806(4)
Np4	O7^{2}	2.387(10)		Cl6	Np5^{2}	2.833(4)
Np4	O1	2.377(11)		O4	Np4^{4}	2.303(10)
Np4	O3	2.385(11)		O4	Np3^{2}	2.201(10)
Np4	O6^{4}	2.406(10)		O1SA	C2SA	1.39(3)
Np4	O5^{2}	2.296(10)		O7	Np4^{1}	2.387(9)
Np2	Np4^{1}	3.7495(9)		O3	Np5^{2}	2.326(10)
Np2	Np5	3.5754(9)		O6	Np7^{7}	2.346(10)
Np2	Cl2	3.022(2)		O6	Np6^{2}	2.353(10)
Np2	Cl1^{4}	2.806(4)		O6	Np4^{4}	2.406(10)
Np2	Cl4	2.850(4)		O1SC	C2SC	1.50(3)
Np2	O2	2.183(10)		O1SB	C2SB	1.49(2)
Np2	O7	2.313(9)		C3SA	C2SA	1.63(3)
Np2	O1	2.319(10)		C4SA	C2SA	1.50(3)
Np2	O1SB	2.381(11)		O5	Np4^{1}	2.296(10)
Np2	O5	2.210(10)		C2SB	C4SB	1.52(3)
Np3	Np4^{1}	3.7470(9)		C2SB	C3SB	1.52(3)
Np3	Np4^{5}	3.7470(9)		C2SC	C3SC	1.53(2)
Np3	Np1^{5}	3.5705(13)		C2SC	C3SC^{4}	1.53(2)

Np3	Cl2	3.040(6)				

[1]+Y,1-X,+Z; [2]1-Y,+X,+Z; [3]1-X,1-Y,+Z; [4]+X,+Y,1-Z; [5]+Y,1-X,1-Z; [6]1-Y,+X,1-Z; [7]1-X,1-Y,1-Z

II.45 $U_2Cl_4(bz)_4(iPrOH)_4$

Table 1 Crystal data and structure refinement for U2Cl4(bz)4(iPrOH)4.	
Identification code	U2Cl4(bz)4(iPrOH)4
Empirical formula	$C_{40}H_{36}Cl_4O_{12}U_2$
Formula weight	1326.55
Temperature/K	296.15
Crystal system	triclinic
Space group	P-1
a/Å	10.683(2)
b/Å	11.322(2)
c/Å	11.736(2)
α/°	67.493(9)
β/°	86.541(10)
γ/°	76.417(10)
Volume/Å^3	1273.9(4)
Z	1
ρ_{calc}g/cm^3	1.729
μ/mm^{-1}	6.608
F(000)	624.0
Crystal size/mm^3	0.177 × 0.142 × 0.118
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.758 to 54.206
Index ranges	-13 ≤ h ≤ 13, -14 ≤ k ≤ 14, -15 ≤ l ≤ 15
Reflections collected	38970
Independent reflections	5582 [R_{int} = 0.0407, R_{sigma} = 0.0302]
Data/restraints/parameters	5582/3/247
Goodness-of-fit on F^2	1.138
Final R indexes [I>=2σ (I)]	R_1 = 0.0304, wR_2 = 0.0888
Final R indexes [all data]	R_1 = 0.0365, wR_2 = 0.0962
Largest diff. peak/hole / e Å^{-3}	1.67/-0.88

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for U2Cl4(bz)4(iPrOH)4. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
U1	3027.4(2)	6130.4(2)	3952.6(2)	26.10(8)
Cl1	1190.3(14)	4910.1(16)	3753.5(17)	43.9(4)

Cl2	1990.6(16)	8662.7(16)	2663.7(18)	53.2(4)
O72A	6223(4)	3010(4)	4772(4)	43.1(10)
O1	1121(4)	6720(4)	5106(5)	42.3(10)
O71B	3318(5)	4475(4)	5896(4)	47.9(11)
O71A	4398(4)	4307(4)	3782(5)	46.5(11)
O72B	5116(4)	3195(4)	6947(5)	51.5(12)
C7B	3918(5)	3507(5)	6782(6)	31.8(12)
C7A	5235(5)	3246(6)	4098(5)	32.3(12)
C1A	5064(5)	2201(6)	3673(6)	36.4(13)
C1B	3144(5)	2674(6)	7717(6)	33.8(12)
O5	2853(6)	6378(7)	1750(7)	79.9(18)
C2A	3899(6)	2337(7)	3128(7)	46.3(16)
C6A	6068(6)	1098(7)	3852(8)	49.8(17)
C4A	4706(8)	238(8)	2959(9)	62(2)
C5A	5882(8)	130(8)	3472(9)	62(2)
C6B	3712(6)	1763(7)	8838(7)	45.7(15)
C5B	2977(8)	1023(8)	9694(8)	67(2)
C2	658(7)	7829(7)	5486(9)	58(2)
C3A	3720(7)	1331(8)	2777(8)	60(2)
C2B	1884(6)	2789(8)	7444(8)	65(2)
C3	-677(8)	8564(9)	4942(11)	80(3)
C4B	1701(9)	1143(11)	9405(11)	100(4)
C4	713(13)	7398(13)	6823(11)	105(4)
C3B	1177(8)	2000(11)	8247(10)	92(4)
C8	4121(18)	6570(19)	-36(18)	153(6)
C7	2030(20)	7850(20)	-310(20)	209(10)
C6	3168(17)	7208(17)	569(17)	137(5)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for U2Cl4(bz)4(iPrOH)4. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	20.70(11)	24.31(12)	31.86(13)	-7.32(8)	-1.25(7)	-7.76(7)
Cl1	32.5(7)	47.6(8)	61.4(10)	-26.5(8)	1.4(7)	-17.5(6)
Cl2	42.7(9)	34.6(8)	60.2(12)	5.3(7)	-6.2(7)	-5.8(6)
O72A	40(2)	42(2)	54(3)	-22(2)	-10(2)	-11.6(19)
O1	32(2)	34(2)	69(3)	-26(2)	13(2)	-12.4(17)
O71B	58(3)	41(2)	36(3)	2(2)	-5(2)	-21(2)
O71A	35(2)	37(2)	75(4)	-32(2)	-4(2)	-2.0(18)
O72B	29(2)	43(3)	74(4)	-11(2)	14(2)	-13.9(19)
C7B	33(3)	28(3)	36(3)	-13(2)	7(2)	-11(2)
C7A	31(3)	40(3)	33(3)	-18(3)	3(2)	-13(2)
C1A	32(3)	36(3)	47(4)	-20(3)	6(2)	-12(2)

C1B	25(3)	35(3)	33(3)	-3(2)	3(2)	-7(2)
C2A	36(3)	52(4)	63(5)	-36(4)	-5(3)	-7(3)
C6A	37(3)	43(4)	74(5)	-28(4)	-5(3)	-6(3)
C4A	64(5)	60(5)	88(6)	-53(5)	3(4)	-22(4)
C5A	55(4)	48(4)	94(7)	-47(5)	-6(4)	0(3)
C6B	35(3)	46(4)	44(4)	-2(3)	-6(3)	-11(3)
C5B	63(5)	64(5)	50(5)	7(4)	-1(4)	-21(4)
C2	42(4)	51(4)	99(7)	-47(5)	20(4)	-22(3)
C3A	50(4)	66(5)	85(6)	-47(5)	-7(4)	-21(4)
C2B	29(3)	72(5)	64(5)	12(4)	-10(3)	-18(3)
C3	41(4)	51(5)	144(10)	-40(6)	16(5)	-4(4)
C4B	61(6)	99(8)	89(8)	31(6)	15(5)	-37(5)
C4	139(11)	132(11)	89(9)	-74(9)	31(7)	-63(9)
C3B	35(4)	103(7)	95(8)	22(6)	1(4)	-36(4)

Table 4 Bond Lengths for U2Cl4(bz)4(iPrOH)4.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
U1	Cl1	2.7185(15)		C1A	C2A	1.383(8)
U1	Cl2	2.6692(16)		C1A	C6A	1.397(9)
U1	O72A[1]	2.335(4)		C1B	C6B	1.388(9)
U1	O1	2.479(4)		C1B	C2B	1.368(8)
U1	O71B	2.313(4)		O5	C6	1.419(19)
U1	O71A	2.303(4)		C2A	C3A	1.406(9)
U1	O72B[1]	2.339(4)		C6A	C5A	1.388(9)
U1	O5	2.505(7)		C4A	C5A	1.385(11)
O72A	U1[1]	2.335(4)		C4A	C3A	1.378(11)
O72A	C7A	1.272(7)		C6B	C5B	1.378(10)
O1	C2	1.460(8)		C5B	C4B	1.387(13)
O71B	C7B	1.253(7)		C2	C3	1.511(12)
O71A	C7A	1.255(7)		C2	C4	1.455(14)
O72B	U1[1]	2.339(4)		C2B	C3B	1.357(11)
O72B	C7B	1.251(7)		C4B	C3B	1.390(14)
C7B	C1B	1.497(8)		C8	C6	1.42(2)
C7A	C1A	1.499(8)		C7	C6	1.50(3)

[1]1-X,1-Y,1-Z