

Fig. S1 Optimized structure for $\text{UO}_2(\text{XDA})(\text{H}_2\text{O})_3$ complex

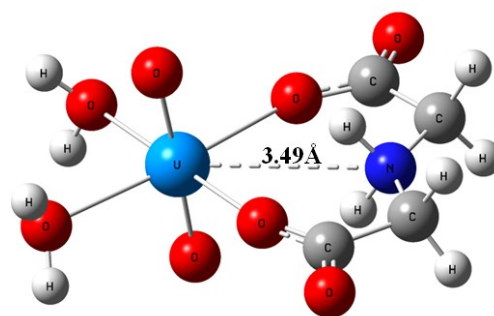
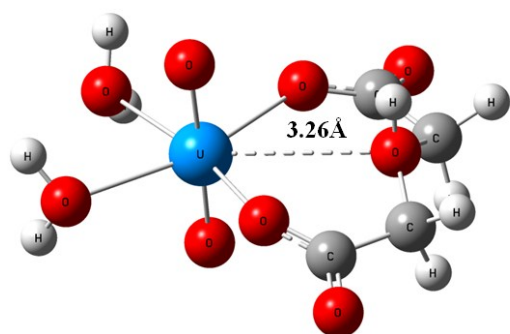


Fig. S2 Optimized structures of O-tri-11 and N-tri-11 after protonation

The U-X bonds are significantly elongated after protonation of the bridging atom.

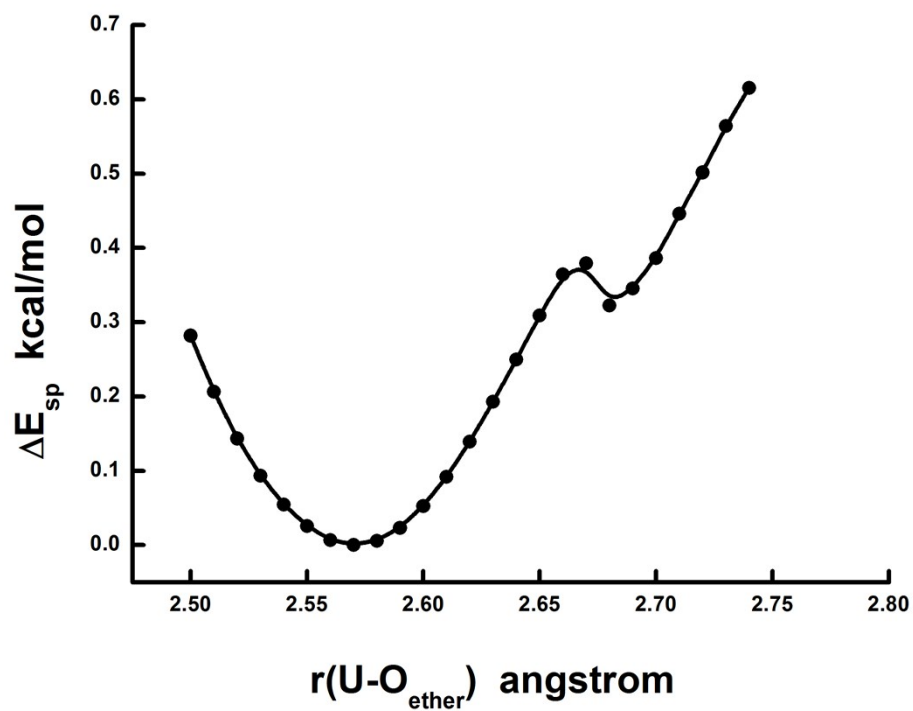


Fig. S3 Potential energy surface scan for O-tri-11 complex in aqueous solutions at B3LYP/ECP60MWB/6-31G(d) level. The U-O_{ether} bond lengths vary between 2.50-2.74Å at the step of 0.01Å.

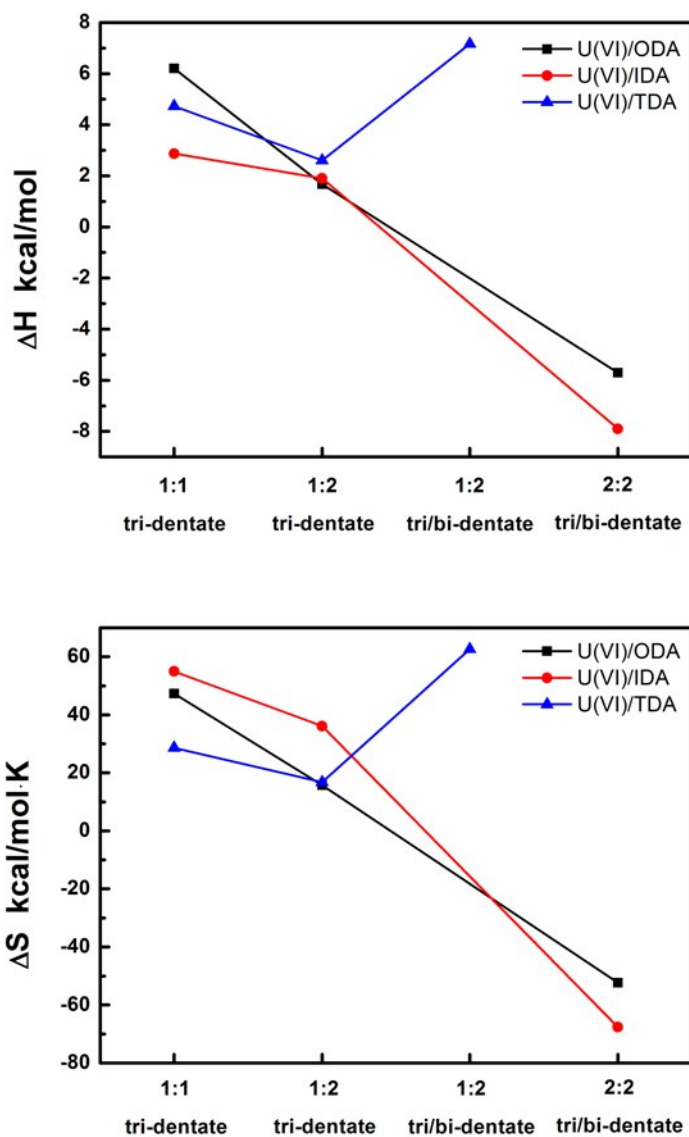


Fig. S4 Enthalpy and entropy trend graphic for U(VI) complexes with ODA, IDA and TDA, respectively

Table S1.

Reaction free energy and enthalpy values in both calculations and experimental studies (aqueous phase; ΔG and ΔH values are in kcal/mol and cal/K·mol)

Mode	ΔH_{cal}	ΔH_{exp}	ΔS_{cal}	ΔS_{exp}
O-tri-11	-22.7	6.21 ¹ , 4.34 ²	58.4	47.3 ¹ , 38.64 ²
N-tri-11	-23.7	2.87 ¹	61.1	54.97 ¹
S-tri-11	-12.8	4.73 ²	56.4	28.66 ²
O-bi-11	0.836	--	64.9	--
N-bi-11	0.168	--	63.4	--
S-bi-11	0.289	--	60.2	--
O-tri-12	-36.1	1.67, 1.76 ²	81.5	16.73, 17.88 ²
N-tri-12	-34.6	1.90 ¹	80.5	36.10 ¹
S-tri-12	-29.5	2.60 ²	72.1	16.78 ²
O-tri/bi-12	-26.7	--	82.6	--
N-tri/bi-12	-30.4	--	84.5	--
S-tri/bi-12	-19.0	7.17 ³ , 6.14 ⁴	78.7	62.62 ³
O-bi-12	-5.15	--	86.7	--
N-bi-12	-6.14	--	87.4	--
S-bi-12	-5.02	--	83.1	--
O-tri-22	-67.2	-5.7 ¹	71.5	-52.3 ¹
N-tri-22	-67.0	-7.9 ¹	74.4	-67.6 ¹
S-tri-22	-57.8	--	67.4	--

1. J. Jiang, J. C. Renshaw, M. J. Sarsfield, F. R. Livens, D. Collison, J. M. Charnock and H. Eccles, *Inorganic Chemistry*, 2003, **42**, 1233-1240.
2. A. Kirishima and N. Sato, *Journal of Chemical Thermodynamics*, 2014, **70**, 227-232.
3. P. Di Bernardo, P. Zanonato, A. Bismondo, H. Jiang, A. Y. Garnov, J. Jiang and L. Rao, *European Journal of Inorganic Chemistry*, 2006, 4533-4540.
4. P. D. Bernardo, G. Tomat, A. Bismondo, O. Traverso and L. Magon, *Journal of Chemical Research (Miniprint)*, 1980, 3044-3071.

Cartesian coordinates of all the complex structures

O-tri-11

O	-1.90381200	0.28868400	-0.12812400
C	-2.42769300	1.59530900	0.10387800
C	-2.82393700	-0.77917400	0.09252600
C	-1.28799100	2.59910300	-0.01413700
H	-2.85986500	1.65813700	1.11109000
H	-3.21088600	1.82731800	-0.62702200
C	-2.06811300	-2.09739900	-0.01988500
H	-3.26453700	-0.69875700	1.09476900
H	-3.63103700	-0.74413400	-0.64837000
O	-0.10714900	2.09037500	-0.19120000
O	-1.53421500	3.80617900	0.06930900
O	-0.78072100	-1.99912100	-0.14898500
O	-2.69749600	-3.15909500	0.02573300
U	0.62646300	-0.12190200	-0.02635000
O	0.49412600	-0.05959400	1.75301300
O	0.81436600	-0.18867100	-1.79926200
O	2.41300500	-1.90706900	0.26019800
H	2.88166600	-1.77301300	1.10397900
H	3.09887600	-1.81756400	-0.42652400
O	2.74582800	1.27024600	0.12710100
H	2.61358100	1.95532000	0.80805300
H	2.83253000	1.76516400	-0.70830400

O-bi-11

O	-3.33438600	-0.37210100	0.03107600
C	-2.38827000	-1.42208500	0.05664400
C	-4.66060100	-0.86250500	0.05513300
C	-0.99097500	-0.85045800	0.05229500
H	-2.49638600	-2.04466300	0.95837800
H	-2.49212100	-2.08465500	-0.81495300
C	-5.66977200	0.26093200	-0.02938500
H	-4.86702500	-1.42485300	0.97727800
H	-4.85408000	-1.53926000	-0.79087000
O	-0.00296700	-1.65430400	-0.05886600
O	-0.77380500	0.39585200	0.16243400
O	-5.12605300	1.47298600	-0.21284000
O	-6.86922700	0.05866900	0.05165400
H	-5.85560700	2.12455100	-0.26268800
U	1.66778700	0.10477700	-0.00339900
O	1.77831200	-0.00034400	1.76117300
O	1.60691400	0.24786700	-1.76851500
O	3.63379600	-1.39523100	-0.17207200
H	3.65765500	-1.87824300	-1.01863600
H	3.64351500	-2.08104800	0.52140700
O	1.57563100	2.58420800	0.14817900
H	1.14019200	2.87306000	0.97145100
H	1.03943900	2.95954900	-0.57458900

O-tri-12

O	2.73751100	0.00043900	-0.08135400
C	3.32256800	1.20072300	-0.56093400
C	3.32334800	-1.19946600	-0.56089200
C	2.47771700	2.34921700	-0.02475300
H	4.35791100	1.29758400	-0.21136200
H	3.32477700	1.22426500	-1.66028400
C	2.47897700	-2.34838000	-0.02493100
H	3.32574400	-1.22299000	-1.66025000
H	4.35867600	-1.29578300	-0.21113900
O	1.35729300	2.00824300	0.51337200
O	2.89906200	3.51198800	-0.13361800
O	1.35758500	-2.00814900	0.51160900
O	2.90153800	-3.51083300	-0.13260000
U	0.01029200	0.00001400	0.16983100
O	-0.20849700	0.00000100	1.94732200
O	0.20749000	-0.00009600	-1.61067100
O	-2.67686000	-0.00045900	-0.21781600
C	-3.44363200	-1.19264000	-0.27532800
C	-3.44412300	1.19141800	-0.27534600
C	-2.48598900	-2.36858300	-0.18009500
H	-4.16224200	-1.23298300	0.55462500
H	-4.00536900	-1.24711300	-1.21744300
C	-2.48695300	2.36777600	-0.18021500
H	-4.00586000	1.24561500	-1.21748500
H	-4.16278000	1.23147100	0.55457100
O	-1.24170700	-2.07120800	-0.03713300
O	-2.94656700	-3.52021600	-0.23943600
O	-1.24239500	2.07083800	-0.03885100
O	-2.94810700	3.51923600	-0.23841800

O-tri/bi-12

O	-3.30239900	0.36716000	0.14622600
C	-3.82764200	1.66935300	-0.10638600
C	-4.21403100	-0.70759600	-0.07796200
C	-2.68175700	2.67570500	-0.08605900
H	-4.31018000	1.69910900	-1.09210500
H	-4.57217900	1.93323200	0.65344800
C	-3.45620500	-2.02423400	0.05449600
H	-5.03228900	-0.67183000	0.65061300
H	-4.64074500	-0.63677300	-1.08705800
O	-1.48708800	2.17293700	-0.01547500
O	-2.94009300	3.88155700	-0.15490100
O	-2.17358400	-1.92412900	0.21616800
O	-4.08457800	-3.08650800	-0.00670100
U	-0.76847000	-0.05052700	0.03531200
O	-0.89332800	-0.13344600	-1.74778300
O	-0.63414500	0.02975500	1.81835800
O	4.26939900	-0.27301300	-0.03551100
C	3.40655000	-1.38356800	-0.19227000
C	5.62851600	-0.63361900	-0.14671200
C	1.96723200	-0.91863300	-0.11399200
H	3.55306200	-1.87176500	-1.16867900
H	3.57595700	-2.14234500	0.58450800
C	6.47315700	0.60781800	0.06881400
H	5.91383500	-1.38752400	0.60362700
H	5.85826900	-1.05336700	-1.13855100
O	1.68047600	0.31934300	-0.16196700
O	1.04929500	-1.79482700	-0.01719900
O	6.02951700	1.70605500	0.33614200
O	7.80585300	0.43047200	-0.04989000
H	8.02397500	-0.49445300	-0.27384500

O-bi-12

C	-6.34451500	0.79405700	0.05162500
C	-4.06934200	1.46185800	0.04700300
C	-7.21160500	-0.43505700	-0.15620900
H	-6.53443100	1.48857700	-0.77913500
H	-6.64738000	1.28671900	0.98466700
C	-2.65835300	0.92010100	0.01198700
H	-4.22349100	2.08603800	-0.84569000
H	-4.17087600	2.10777100	0.92970400
O	-6.55577500	-1.57511400	-0.42452100
O	-8.42676500	-0.39997600	-0.10249800
O	-2.42978400	-0.32358300	-0.12067900
O	-1.68922900	1.74252100	0.12170400
U	0.01514200	-0.03081500	0.05225000
O	0.11180700	0.12420900	-1.71400000
O	-0.08219300	-0.18629500	1.81830900
H	-5.59257400	-1.38226000	-0.41477300
C	4.11283400	-1.48458700	0.01459100
C	6.36675400	-0.71528400	-0.05510300
C	2.69609200	-0.96179600	0.09396500
H	4.22889500	-2.31196000	0.72699800
H	4.26338900	-1.88938500	-0.99691400
C	7.11213100	0.60069100	-0.19610000
H	6.86282700	-1.32782000	0.70752700
H	6.43567600	-1.24255300	-1.01707300
O	2.45697600	0.27861000	0.23940100
O	1.73388500	-1.79106400	-0.02467300
O	6.34603700	1.70262100	-0.21109800
O	8.32173400	0.66493100	-0.31325100
H	5.41107500	1.41780500	-0.10204400
O	-4.98761900	0.38591600	0.08708200
O	5.01965400	-0.43250500	0.28536800

O-tri-22

O	4.48994500	0.01421400	-0.10935300
C	5.23630900	1.22385600	-0.19550500
C	5.25848300	-1.18191800	-0.19552300
C	4.27064000	2.40091600	-0.10737600
H	5.78263000	1.26794800	-1.14646200
H	5.96335900	1.28291900	0.62443400
C	4.31141700	-2.37580900	-0.13245200
H	5.81794000	-1.20875000	-1.13950500
H	5.97535400	-1.23519500	0.63361400
O	3.01883200	2.10340700	0.01848800
O	4.73207800	3.54891700	-0.15779300
O	3.05145800	-2.09959800	-0.04592100
O	4.79321400	-3.51602200	-0.16712600
U	1.91792900	-0.00794300	0.04245200
O	1.79381000	0.04074800	-1.75251900
O	2.03513400	-0.05979600	1.83782600
O	-4.51187300	0.01919100	-0.03324000
C	-5.22922600	-1.17004700	-0.35619800
C	-5.19929100	1.23107100	-0.33548200
C	-4.30906400	-2.37043900	-0.16101400
H	-5.56025500	-1.14111000	-1.40337100
H	-6.11348700	-1.26687900	0.28429600
C	-4.25562700	2.40504200	-0.09721200
H	-5.51673200	1.23522700	-1.38717800
H	-6.08974300	1.33163900	0.29586300
O	-3.05843200	-2.10167200	0.02820300
O	-4.79589700	-3.50763600	-0.21398800
O	-3.01830500	2.10278600	0.12441300
O	-4.71349600	3.55443800	-0.14739100
U	-1.92355300	-0.01208400	0.09640400
O	-1.83494900	0.05230300	-1.70037100
O	-2.00945900	-0.07902100	1.89320800
H	-0.01199400	1.93754600	-0.59526900
H	0.01502200	-1.81565100	1.03412700
O	-0.00250600	1.39821100	0.21601300
O	-0.00036500	-1.41062600	0.14821000

N-tri-11

C	-2.81762100	-0.54599900	-0.21611100
C	-2.16262100	1.84518000	-0.23874100
C	-2.21275700	-1.92915100	0.01434100
H	-2.92550500	-0.41173800	-1.29878000
H	-3.81928700	-0.49353000	0.22466000
C	-0.95844100	2.74622500	0.02881800
H	-2.28640600	1.77074300	-1.32529200
H	-3.07161000	2.30357100	0.16697800
O	-0.93137900	-1.93644100	0.24792600
O	-2.91645900	-2.94174100	-0.05613500
O	0.13745500	2.11827600	0.35109800
O	-1.05397600	3.97176500	-0.08982700
U	0.58612600	-0.15968300	0.04907600
O	0.24797700	-0.01830600	-1.69928400
O	0.95135200	-0.29884400	1.79472000
O	2.88840700	0.83686900	-0.35650700
H	2.79942600	1.52997900	-1.03669000
H	3.14518100	1.31811200	0.45161300
O	2.08084300	-2.20322900	-0.39831700
H	2.54422900	-2.06425800	-1.24408400
H	2.78795400	-2.20407500	0.27240900
N	-1.91469500	0.49719500	0.29733000
H	-2.01978700	0.53731700	1.31367500

N-bi-11

C	-2.47806400	-1.30570100	0.18359700
C	-4.80370800	-0.71343300	0.16976900
C	-1.06171200	-0.80217900	0.07906500
H	-2.58953700	-1.69454100	1.21360000
H	-2.58889800	-2.16570700	-0.48377700
C	-5.86479500	0.33834200	-0.05780700
H	-4.91608400	-1.03433700	1.22222600
H	-5.06866900	-1.57768500	-0.44570000
O	-0.09619600	-1.62985000	-0.05970800
O	-0.79854400	0.44251500	0.17235600
O	-5.39901100	1.59690600	0.05353900
O	-7.03843600	0.08094800	-0.26746300
H	-6.15042400	2.21070900	-0.07581700
U	1.61808900	0.09221500	-0.01503800
O	1.72717700	-0.02591900	1.74978000
O	1.55827000	0.23687900	-1.78100700
O	3.52029700	-1.46530000	-0.17489200
H	3.53642100	-1.94956900	-1.02112500
H	3.51301100	-2.15016400	0.51985300
O	3.05390000	2.10951600	0.12039600
H	2.95251000	2.59110700	0.96193000
H	2.86414600	2.75994500	-0.58076200
N	-3.44974700	-0.26991000	-0.15609100
H	-3.23846100	0.54811900	0.41394500

N-tri-12

C	-3.21810200	1.36593000	0.10944500
C	-3.35947700	-1.08618700	0.26840100
C	-2.27542800	2.47285300	-0.33614900
H	-3.29775400	1.40256800	1.19891300
H	-4.21631400	1.53930700	-0.30289300
C	-2.53651000	-2.33917700	0.01299400
H	-3.45867100	-0.95934200	1.34956200
H	-4.36486100	-1.21008600	-0.14416700
O	-1.09259800	2.09820500	-0.64402500
O	-2.68372300	3.64884200	-0.37348500
O	-1.31277900	-2.14396100	-0.30476200
O	-3.07026700	-3.45807400	0.12973400
U	-0.00190500	-0.04491200	0.03673800
O	-0.43719800	-0.03688000	1.77489800
O	0.40622000	-0.08571300	-1.70692800
N	-2.65740200	0.07255600	-0.28499500
H	-2.69259200	0.00808500	-1.30067500
C	3.21582300	1.28312300	-0.29048800
C	3.25531400	-1.17948400	-0.47687300
C	2.37323700	2.40377900	0.30311300
H	3.15226800	1.34185000	-1.38014900
H	4.26506900	1.41616200	-0.01123400
C	2.45999700	-2.40524800	-0.04945400
H	3.17982700	-1.08130300	-1.56282600
H	4.31173700	-1.31534900	-0.22755000
O	1.22524300	2.05304900	0.74074800
O	2.82575200	3.56464000	0.32928800
O	1.29903100	-2.17041000	0.43571400
O	2.95637500	-3.53886300	-0.19098900
N	2.66734000	0.00203900	0.15289600
H	2.80942900	-0.07234100	1.15835400

N-tri/bi-12

C	-4.14202600	-0.81018200	-0.39727100
C	-3.76681900	1.64316400	-0.42761300
C	-3.37924100	-2.11102100	-0.14742100
H	-4.22058500	-0.68368500	-1.48330000
H	-5.16031800	-0.89301000	-0.00096600
C	-2.68850600	2.68104000	-0.11877200
H	-3.81661200	1.53462900	-1.51719200
H	-4.74332500	2.00766000	-0.08828900
O	-2.12479600	-1.97102500	0.16943800
O	-3.94911300	-3.19978600	-0.28084700
O	-1.54839100	2.19338000	0.28061700
O	-2.91774700	3.88488900	-0.27686000
U	-0.82128900	-0.02678100	0.13576300
O	-0.97416300	0.04577300	-1.64939600
O	-0.70244100	-0.09385300	1.92442000
N	-3.40977400	0.34013300	0.15673100
H	-3.59224900	0.38230800	1.16153800
C	3.37600400	-1.32250000	-0.20918100
C	5.68649200	-0.66716800	-0.18654900
C	1.94006200	-0.86359000	-0.09244300
H	3.50609000	-2.19397100	0.44097300
H	3.50310500	-1.69074400	-1.24458600
C	6.63190300	0.50469900	-0.08432400
H	6.03370700	-1.46235300	0.48212300
H	5.79083200	-1.06360600	-1.21369100
O	1.65288700	0.37674600	-0.04077000
O	1.01176700	-1.73659000	-0.07879400
O	6.29688400	1.67387000	-0.00278700
O	7.92127000	0.11184700	-0.13620300
N	4.32538100	-0.27689000	0.15462400
H	4.09381300	0.55910200	-0.38068800
H	8.47838900	0.91613300	-0.11471700

N-bi-12

C	6.45962500	-0.15210900	-0.00537000
C	4.28002200	-1.14744700	-0.17089600
C	7.29026100	1.10713500	0.08120500
H	6.90469800	-0.78125400	-0.78169900
H	6.62149300	-0.68146900	0.95267300
C	2.79171200	-0.89867300	-0.18774700
H	4.52027700	-1.83444700	-0.99003700
H	4.48805000	-1.70141300	0.76300900
O	6.57216000	2.20321400	0.39112300
O	8.50174000	1.12695400	-0.05972300
O	2.32401800	0.28829900	-0.12744800
O	1.98343900	-1.88595400	-0.20883000
U	-0.01273200	-0.42817500	0.01194800
O	-0.14525500	-0.36862300	-1.75945300
O	0.11460700	-0.50402000	1.78295100
N	5.04912200	0.08683700	-0.29988500
H	4.69032800	0.74454000	0.39074100
H	7.19226600	2.95709200	0.46489900
C	-3.93681500	1.44055700	-0.08095600
C	-6.31400700	1.12689900	-0.52495300
C	-2.60408600	0.74969600	0.08325100
H	-4.06782100	2.13802400	0.75386700
H	-3.85814200	2.05281100	-0.99344300
C	-7.49981100	0.34767400	0.02482700
H	-6.37224600	2.13166600	-0.09014200
H	-6.43532400	1.23717800	-1.60942400
O	-2.50682200	-0.51783000	0.10672100
O	-1.54447800	1.46512000	0.14846400
O	-7.18114900	-0.52873200	0.98986300
O	-8.65149700	0.50931000	-0.34143000
N	-5.05352700	0.49619900	-0.11969000
H	-4.82553300	-0.23616800	-0.79132500
H	-6.19141500	-0.46005600	1.07463400

N-tri-22

C	-5.17599700	-1.22598200	0.30315400
C	-5.14692100	1.25026600	0.34206700
C	-4.24917700	-2.41394200	0.04579100
H	-6.17201200	-1.43663500	-0.10384400
H	-5.28151400	-1.12558400	1.38997900
C	-4.21119000	2.42981200	0.07962600
H	-6.15056100	1.48163700	-0.03433600
H	-5.22504300	1.13019700	1.42923000
O	-3.01437900	-2.11358500	-0.21272400
O	-4.69072000	-3.56893300	0.12404100
O	-2.99548700	2.11564800	-0.24429000
O	-4.62705300	3.58940800	0.21191000
U	-1.92228100	-0.00543000	-0.14334900
O	-1.81004500	-0.04403200	-1.94333800
O	-2.07862200	0.02732900	1.65240000
C	5.15337900	1.23195200	-0.36681200
C	5.16601700	-1.24371500	-0.29221300
C	4.22431000	2.42061600	-0.12262600
H	5.22962500	1.09457100	-1.45213200
H	6.15861800	1.46339200	0.00509300
C	4.23385300	-2.42238100	-0.01220800
H	5.26641700	-1.16000100	-1.38083200
H	6.16299200	-1.45474200	0.11241200
O	3.00266400	2.11820900	0.19031700
O	4.65062000	3.57598000	-0.25834600
O	3.00799400	-2.11018700	0.27284600
O	4.66330100	-3.58144200	-0.09734200
U	1.92280200	0.00052400	0.14589600
O	2.07692600	-0.04802300	-1.64968600
O	1.81308100	0.05560400	1.94568200
H	0.07740000	-1.87486900	-0.83068600
H	-0.07616800	1.86811700	0.83627100
O	0.00434500	-1.41213900	0.02341400
O	-0.00390500	1.40621500	-0.01832300
N	4.59325900	0.00778900	0.22262700
H	4.75049600	0.04072100	1.23132200
N	-4.59285300	0.01384900	-0.22734000
H	-4.74643900	0.03293400	-1.23700500

S-tri-11

C	-2.40663600	1.78336600	-0.25417100
C	-2.83422700	-1.10375300	-0.22115100
C	-1.14995000	2.66118800	-0.17367500
H	-3.27902700	2.35827000	0.06130300
H	-2.55343800	1.47408000	-1.29459900
C	-1.84730500	-2.27897100	-0.20387200
H	-3.80543600	-1.43553500	0.15086100
H	-2.96010100	-0.76711000	-1.25582900
O	-0.06142000	2.07660300	0.23741500
O	-1.22476700	3.84580400	-0.50472800
O	-0.63835700	-2.01883700	0.20081300
O	-2.23687300	-3.38818700	-0.57464100
U	0.70857700	-0.11453200	0.06628500
O	1.08748100	-0.18016200	1.80785900
O	0.29259000	-0.04649800	-1.66689300
O	2.51276800	-1.86816400	-0.31128000
H	3.21076900	-1.75358700	0.35936700
H	2.95770200	-1.71141600	-1.16423900
O	2.81390400	1.28192100	-0.38293200
H	2.85258500	1.97919000	0.29770500
H	2.66501300	1.76378700	-1.21704300
S	-2.20068800	0.28990500	0.78978700

S-bi-11

C	2.19914000	-1.19362700	-0.02182700
C	4.90734000	-0.79233400	0.14333600
C	0.77052400	-0.71320700	-0.05940700
H	2.36452200	-1.85156700	-0.88292200
H	2.33266400	-1.79517700	0.88391500
C	6.17065500	0.02649600	0.00870500
H	4.93969300	-1.58224500	-0.61006200
H	4.92212700	-1.26417900	1.13357900
O	-0.17556100	-1.56554300	0.06961400
O	0.47764900	0.51386000	-0.20536900
O	6.03889900	1.28673300	0.46061000
O	7.21466000	-0.41829800	-0.43367700
H	6.89879100	1.74219200	0.35055400
U	-1.94857700	0.06657100	-0.00445500
O	-2.07181100	-0.05272700	-1.76722600
O	-1.87790500	0.22614400	1.75863600
O	-3.96567500	-1.35616200	0.23265900
H	-3.98331400	-1.83314000	1.08280000
H	-4.03311500	-2.04392100	-0.45544800
O	-1.86062500	2.54469300	-0.16514700
H	-1.43074100	2.82057300	-0.99596900
H	-1.30558400	2.91359200	0.54663700
S	3.37756800	0.21098900	-0.04180600

S-tri-12

C	-4.03170000	-1.41663000	-0.17526300
C	-4.03141900	1.41716200	-0.17563500
C	-2.65699200	-1.67842400	0.46032500
H	-4.28482700	-2.29736100	-0.77861200
H	-4.77571800	-1.34066800	0.62187100
C	-2.65663700	1.67855600	0.45992300
H	-4.28419500	2.29780200	-0.77925300
H	-4.77554000	1.34161900	0.62145100
O	-1.60966900	-1.46419900	-0.27346700
O	-2.63205900	-2.13869900	1.61196700
O	-1.60942000	1.46434000	-0.27408600
O	-2.63142000	2.13835400	1.61173000
U	0.21407500	0.00009200	0.01113100
O	0.57948500	-0.00006300	-1.74990000
O	-0.02142600	0.00024400	1.78958000
S	-4.19956700	0.00012500	-1.32260600
C	3.65732700	-1.45353000	-0.28356800
C	3.65783600	1.45306700	-0.28301200
C	2.53089100	-2.49779500	-0.25385000
H	4.58845100	-1.91047100	0.05664900
H	3.79651100	-1.12223300	-1.31837500
C	2.53151300	2.49746000	-0.25353800
H	4.58885800	1.90985400	0.05769300
H	3.79744200	1.12202300	-1.31784200
O	1.35275400	-2.08207400	0.08338400
O	2.80267100	-3.66359000	-0.56676800
O	1.35322700	2.08188500	0.08336600
O	2.80353200	3.66323200	-0.56633000
S	3.23380200	-0.00035500	0.75036900

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C	-3.84970500	1.94778800	-0.55809800
C	-4.41281500	-0.91488800	-0.67632900
C	-2.58356000	2.76146800	-0.24887900
H	-3.82813400	1.66129800	-1.61502300
H	-4.73472600	2.56309900	-0.38652500
C	-3.52329500	-2.15378200	-0.49320700
H	-5.45749400	-1.18464300	-0.51167000
H	-4.30686900	-0.55988800	-1.70719000
O	-1.60840600	2.12271200	0.32930600
O	-2.54718500	3.95104800	-0.57183200
O	-2.36413400	-1.96258800	0.06486300
O	-3.93515900	-3.24534400	-0.89322400
U	-0.93918700	-0.11878700	0.22576600
O	-1.09601000	0.02874200	-1.54934200
O	-0.86262400	-0.24913700	2.00865300
C	3.32379100	-1.10823000	-0.04161500
C	5.99956800	-0.60004400	-0.08831500
C	1.86452500	-0.71624900	0.00193400
H	3.47740800	-1.76944900	-0.90112100
H	3.53885600	-1.69087600	0.86166600
C	7.19000200	0.32523900	-0.18745600
H	6.07392100	-1.17257100	0.84395800
H	6.04491300	-1.31786100	-0.91629400
O	1.49637300	0.49856900	0.06492500
O	0.99510900	-1.65033600	-0.00502900
O	7.12758400	1.53331100	-0.31345900
O	8.39912700	-0.27481200	-0.12906000
H	8.30792300	-1.24125100	-0.02569100
S	-3.90838600	0.42683800	0.46929500
S	4.43344600	0.34662400	-0.13849400

S-bi-12

C	-6.34451500	0.79405700	0.05162500
C	-4.06934200	1.46185800	0.04700300
C	-7.21160500	-0.43505700	-0.15620900
H	-6.53443100	1.48857700	-0.77913500
H	-6.64738000	1.28671900	0.98466700
C	-2.65835300	0.92010100	0.01198700
H	-4.22349100	2.08603800	-0.84569000
H	-4.17087600	2.10777100	0.92970400
O	-6.55577500	-1.57511400	-0.42452100
O	-8.42676500	-0.39997600	-0.10249800
O	-2.42978400	-0.32358300	-0.12067900
O	-1.68922900	1.74252100	0.12170400
U	0.01514200	-0.03081500	0.05225000
O	0.11180700	0.12420900	-1.71400000
O	-0.08219300	-0.18629500	1.81830900
H	-5.59257400	-1.38226000	-0.41477300
C	4.11283400	-1.48458700	0.01459100
C	6.36675400	-0.71528400	-0.05510300
C	2.69609200	-0.96179600	0.09396500
H	4.22889500	-2.31196000	0.72699800
H	4.26338900	-1.88938500	-0.99691400
C	7.11213100	0.60069100	-0.19610000
H	6.86282700	-1.32782000	0.70752700
H	6.43567600	-1.24255300	-1.01707300
O	2.45697600	0.27861000	0.23940100
O	1.73388500	-1.79106400	-0.02467300
O	6.34603700	1.70262100	-0.21109800
O	8.32173400	0.66493100	-0.31325100
H	5.41107500	1.41780500	-0.10204400
O	-4.98761900	0.38591600	0.08708200
O	5.01965400	-0.43250500	0.28536800

S-tri-22

C	-5.34927500	1.45996400	0.22479400
C	-5.34892000	-1.44787100	0.25562500
C	-4.21325300	2.49406600	0.17948500
H	-5.47850100	1.13329900	1.26243800
H	-6.27938200	1.92808200	-0.10278100
C	-4.21802300	-2.48765200	0.21760100
H	-5.46552300	-1.10156400	1.28844100
H	-6.28450500	-1.91666400	-0.05467500
O	-3.04190500	2.06963600	-0.17291500
O	-4.47098100	3.66178000	0.49626200
O	-3.04431300	-2.06988100	-0.13659600
O	-4.48020600	-3.65240800	0.54059500
U	-1.89777200	-0.00295800	-0.13627400
O	-2.09447800	0.02582600	1.65166500
O	-1.73665300	-0.03328600	-1.92651700
C	5.22994800	1.44467600	-0.59760500
C	5.21984100	-1.47067800	-0.57704100
C	4.15637700	2.50636900	-0.31343500
H	5.12890200	1.11883100	-1.63862800
H	6.22267100	1.87893100	-0.46750900
C	4.13760500	-2.52012600	-0.28056500
H	5.12357300	-1.15826500	-1.62260100
H	6.20882600	-1.91119400	-0.43939600
O	3.05600400	2.09136700	0.23150200
O	4.38494300	3.67902800	-0.63163000
O	3.04529600	-2.09164800	0.26904900
O	4.35349700	-3.69652700	-0.59471500
U	1.93058800	0.00581900	0.23836500
O	1.80937200	0.04380500	2.03265100
O	2.13589400	-0.02497100	-1.54769800
H	-0.08078100	1.86140300	0.89607600
H	0.11047800	-1.85985200	-0.78633700
O	0.00981700	1.40034300	0.04238200
O	0.01722700	-1.39730400	0.06625100
S	5.00136100	-0.00437300	0.50179200
S	-4.96753500	-0.00530000	-0.81072300