

Complexation of Pu(VI) with N,N,N',N'-tetramethyl-3-oxa-glutar-amide (TMOGA) and related ligands: optical properties and coordination modes

Lei Xu[§], Ning Pu[§], Taoxiang Sun, Youzhen Li, Pingping Wei, Jing Chen*, Chao Xu*

Collaborative Innovation Center of Advanced Nuclear Energy Technology, Institute of Nuclear and New Energy Technology, Tsinghua University, Beijing 100084, China

Supplementary Information

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1. The fitted absorbance data at two representative wavelengths for the complexation of Pu(VI) with TMOGA, DMOGA and ODA.

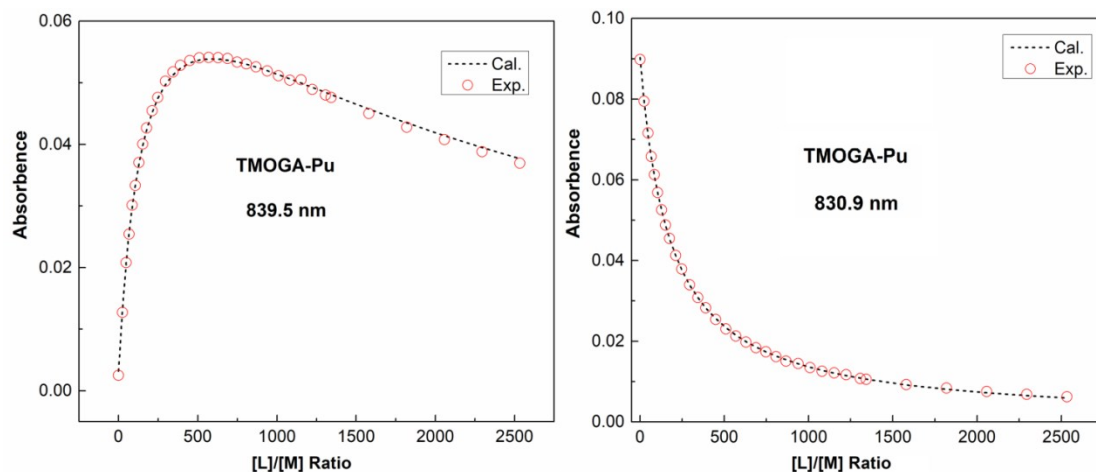


Figure S1. The fitted absorbance data for the complexation of Pu(VI) with TMOGA at two representative wavelengths in 1.0 M NaClO₄ solution at 298K. (Cycles – experimental absorbance, dashed line – calculated absorbance)

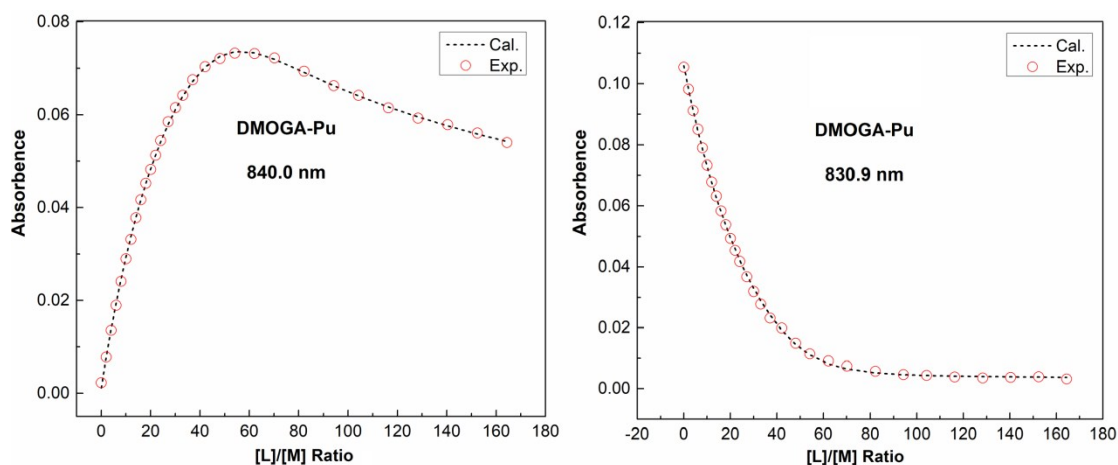


Figure S2. The fitted absorbance data for the complexation of Pu(VI) with DMOGA at two representative wavelengths in 1.0 M NaClO₄ solution at 298K. (Cycles – experimental absorbance, dashed line – calculated absorbance)

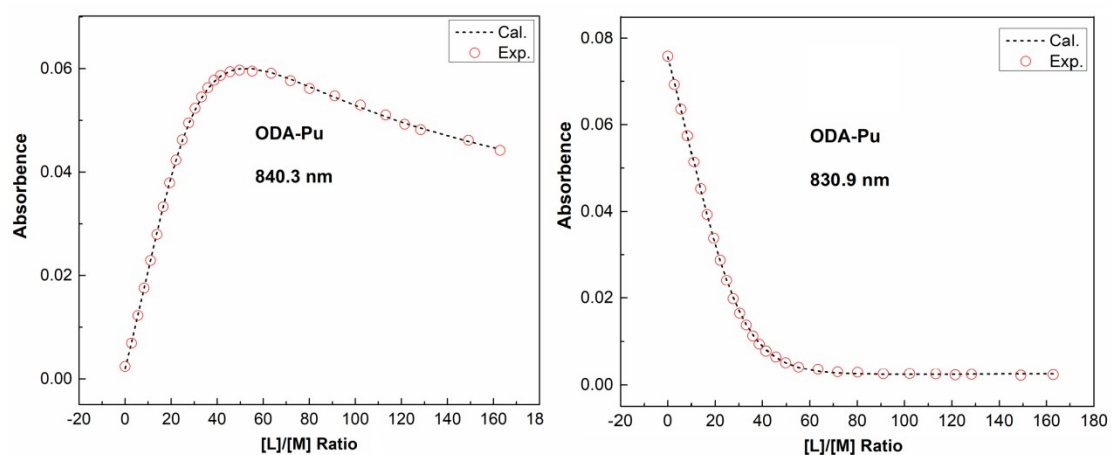


Figure S3. The fitted absorbance data for the complexation of Pu(VI) with ODA at two representative wavelengths in 1.0 M NaClO₄ solution at 298K. (Circles – experimental absorbance, dashed line – calculated absorbance)

2. The ¹H NMR spectrum of ligand TMOGA in D₂O

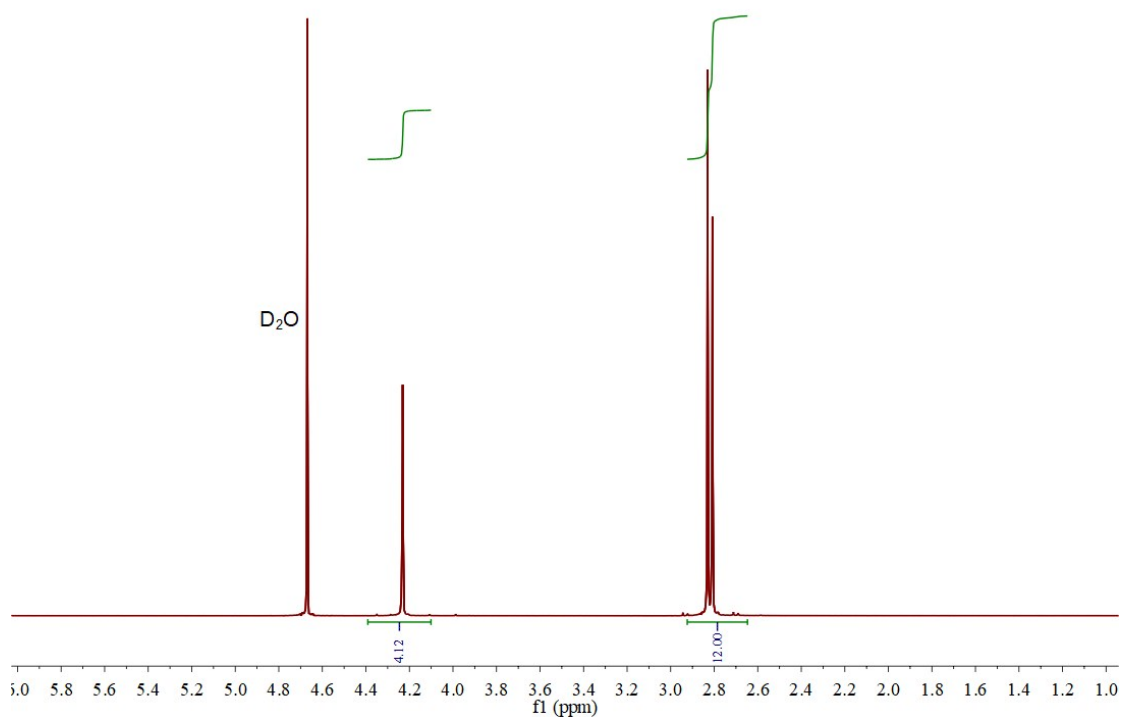


Figure S4. The ¹H NMR spectrum of ligand TMOGA (600 MHz, D₂O)

3. The coordinates of the optimized structures of Pu(VI) complexes by DFT methods.

Pu(VI)/5H₂O

O	0.26678000	2.45087700	-0.00004100
O	-1.65354200	-1.82772000	0.00159300
O	-2.24979300	1.00720100	-0.00169400
O	0.00063000	0.00141900	1.71573500
O	-0.00208400	-0.00040600	-1.71529000
Pu	-0.00020000	0.00015300	0.00019500
O	1.22778300	-2.13671000	-0.00143200
H	1.18703500	-2.82751700	-0.68784000
H	1.84297300	-2.45220300	0.68561800
O	2.41285500	0.50279500	-0.00061700
H	3.05677300	0.25373300	-0.68863700
H	2.90142100	0.99700900	0.68280300
H	0.69192900	2.98853100	-0.69305500
H	-2.62617900	1.58563000	-0.69004800
H	-2.32191900	-2.00449700	-0.68548200
H	-2.92938300	0.90677300	0.68978600
H	-1.76565900	-2.50746400	0.69111100
H	-0.03921800	3.06596200	0.69141700

1:1 Pu(VI)/TMOGA-2H₂O

O	1.55392800	-2.88361700	0.00093500
O	-1.55393200	-2.88371300	-0.00050300
C	2.34792200	1.36080600	0.00016100
C	1.19786400	2.36526400	0.00012400
O	2.03428100	0.13185600	0.00019700
C	-1.19785500	2.36530300	0.00037800
C	-2.34792700	1.36085700	-0.00008800
O	-2.03422800	0.13191900	-0.00048400
O	-0.00000500	1.58913900	-0.00024100
H	1.23234000	3.00169600	0.89388300
H	1.23267900	3.00205400	-0.89336200
H	-1.23259300	3.00247100	-0.89283900
H	-1.23237300	3.00135500	0.89440800
O	-0.00038000	-1.02234800	1.71855800
O	0.00037700	-1.02291200	-1.71851800
N	3.60168200	1.77757300	0.00025000
C	4.72002800	0.81814700	-0.00026800
H	4.33279000	-0.19774000	0.00023900

H	5.33120900	0.98284900	-0.89229200
H	5.33234900	0.98332100	0.89086900
C	4.00168900	3.19367000	-0.00063000
H	4.60030900	3.39728900	-0.89336200
H	3.13992000	3.85928400	0.00393000
H	4.60799400	3.39576500	0.88719900
Pu	-0.00000500	-0.99727900	0.00001300
N	-3.60168900	1.77758500	-0.00015800
C	-4.00170700	3.19367400	0.00071000
H	-3.13992900	3.85929400	0.00230600
H	-4.60325700	3.39739100	-0.89000400
H	-4.60509400	3.39567300	0.89057100
C	-4.72000800	0.81813400	-0.00065500
H	-5.33344000	0.98566100	-0.89058300
H	-4.33275200	-0.19774100	-0.00438600
H	-5.33008700	0.98044900	0.89256600
H	1.95826900	-3.29166400	0.78664400
H	1.95850200	-3.29246500	-0.78422200
H	-1.95854600	-3.29240300	0.78473200
H	-1.95807500	-3.29214700	-0.78611300

1:1 Pu(VI)/DMOGA-2H₂O

C	2.53503700	0.19190100	0.01928300
C	2.05649700	1.64345400	-0.01860400
O	1.66307900	-0.71588200	0.07325100
C	-0.01609300	2.88268400	0.00430300
C	-1.53231700	2.64616500	-0.00571000
O	-2.28943400	3.57771500	-0.14017200
O	-1.87476800	1.37966400	0.15448000
O	0.64714200	1.60611300	0.10938500
H	2.49472800	2.22552700	0.80299400
H	2.34057200	2.11546600	-0.97016600
H	0.28125500	3.38167900	-0.92518700
H	0.25672700	3.51495000	0.85678800
O	-0.78608100	-0.70722700	1.74129800
O	-0.63436100	-0.41579500	-1.70854900
N	3.83870300	-0.07544900	-0.00706900
C	4.31965300	-1.46220900	0.04380800
H	3.47291600	-2.13720500	0.14316600
H	4.87036900	-1.69102700	-0.87404800
H	4.98938700	-1.58028300	0.90130800

C	4.88881800	0.94638900	-0.06689200
H	5.56323800	0.71724600	-0.89750000
H	4.47646300	1.94150600	-0.22565600
H	5.46429500	0.94383000	0.86487300
Pu	-0.71791400	-0.51272600	0.01947300
O	-0.79444400	-2.98866500	-0.25415000
H	-0.96647300	-3.43486900	-1.10009700
H	-0.75171300	-3.67174300	0.43491300
O	-3.20846500	-0.91538400	-0.11569900
H	-3.49067100	0.02002800	-0.18348300
H	-3.67896900	-1.27533200	0.65525600

1:1 Pu(VI)/ODA-2H₂O

C	2.40371600	1.59140500	0.01546700
C	1.21721000	2.56699700	0.06970600
O	2.05521500	0.33646900	-0.16039000
C	-1.21804900	2.56671900	0.06958200
C	-2.40425800	1.59070400	0.01623500
O	-3.53616500	2.01378100	0.13509000
O	-2.05553200	0.33578400	-0.15906800
O	-0.00031400	1.84101700	-0.12883900
H	1.20370300	3.06240900	1.04918300
H	1.33076800	3.33160600	-0.70790300
H	-1.33201700	3.33082700	-0.70845100
H	-1.20446400	3.06267100	1.04877500
O	0.00042300	-0.51795400	1.68476600
O	-0.00023100	-0.82566000	-1.78089400
Pu	0.00006500	-0.62964300	-0.05624400
O	3.53556100	2.01470000	0.13406000
O	-1.92567300	-2.30098300	0.21626500
H	-2.57205500	-1.58811000	0.01148400
H	-2.11201100	-2.54985000	1.13686200
O	1.92723200	-2.30038800	0.21864900
H	2.11139100	-2.54530200	1.14075700
H	2.57271300	-1.58688900	0.01320200

2:1 Pu(VI)/TMOGA

C	2.32216000	2.51781400	-0.05991600
C	1.19248200	3.47159400	0.31702300
O	2.02525600	1.31842800	-0.28287100
C	-1.18925100	3.47308800	0.31916600
C	-2.32105200	2.52033700	-0.05385800

O	-2.02654100	1.32027300	-0.27620600
O	0.00095900	2.72160200	0.15243100
H	1.29636500	3.81450600	1.35669700
H	1.18166100	4.34949700	-0.34219000
H	-1.17914100	4.35027000	-0.34101900
H	-1.29005700	3.81725300	1.35869200
O	-0.00111900	0.16508000	1.71706400
O	-0.00092900	-0.16653200	-1.72000900
N	3.56784400	2.98050300	-0.15103500
C	4.66209300	2.09617700	-0.56997600
H	4.25338700	1.12981100	-0.85724600
H	5.18044000	2.54649700	-1.42208600
H	5.37277400	1.97414900	0.25403900
C	3.94944200	4.37410200	0.10633000
H	4.18090700	4.88470500	-0.83479100
H	3.16225000	4.91807400	0.62732700
H	4.84110100	4.38393700	0.73939200
Pu	-0.00090200	-0.00059600	-0.00147100
N	-3.56622300	2.98482200	-0.14320600
C	-3.94488200	4.37956700	0.11211800
H	-3.15777700	4.92175900	0.63514900
H	-4.17249800	4.89029400	-0.82988000
H	-4.83824400	4.39199100	0.74270200
C	-4.66251700	2.10180800	-0.55968800
H	-5.18330100	2.55376100	-1.40943700
H	-4.25541200	1.13563400	-0.84977900
H	-5.37061300	1.97894700	0.26645400
C	2.32167600	-2.51834000	0.06232100
C	1.19117000	-3.47459100	-0.30639000
O	2.02473700	-1.31820300	0.28096000
C	-1.19001700	-3.47653300	-0.30859800
C	-2.32141600	-2.52060200	0.05674600
O	-2.02540000	-1.32010300	0.27545000
O	-0.00027500	-2.72325100	-0.14811100
H	1.29460100	-3.82631500	-1.34309400
H	1.18023500	-4.34689400	0.36021200
H	-1.17988800	-4.34830500	0.35875600
H	-1.29102000	-3.82903800	-1.34527600
N	3.56812000	-2.97957900	0.15073900
C	4.66342700	-2.09198000	0.55991900
H	4.25503700	-1.12426900	0.84307000
H	5.18580700	-2.53682800	1.41250800
H	5.37047200	-1.97430900	-0.26793800
C	3.94979300	-4.37441000	-0.09969000

H	4.18628200	-4.87876300	0.84356500
H	3.16055000	-4.92243400	-0.61325900
H	4.83842700	-4.38754800	-0.73698900
N	-3.56763600	-2.98237600	0.14322000
C	-3.94777100	-4.37795600	-0.10550400
H	-3.15745300	-4.92603600	-0.61737000
H	-4.18476000	-4.88105700	0.83828100
H	-4.83568200	-4.39283400	-0.74368600
C	-4.66422500	-2.09480800	0.54914100
H	-5.18981200	-2.54058300	1.39921100
H	-4.25674300	-1.12745500	0.83496400
H	-5.36804200	-1.97600300	-0.28126100

2:1 Pu(VI)/DMOGA

Title Card Required

C	2.63426000	1.56198200	-0.01521300
C	3.55556900	0.83962100	-1.01198200
O	1.39673700	1.48027700	-0.12257600
C	3.04312700	-1.25080400	-2.02876900
C	2.63800700	-2.06535500	-0.78286900
O	2.98678100	-3.22925500	-0.71975400
O	1.94867200	-1.41886100	0.13343700
O	2.80415700	0.14993600	-1.96720500
H	4.17834200	1.59202500	-1.52101900
H	4.23092500	0.17518400	-0.45653000
H	4.09815700	-1.46643000	-2.24815600
H	2.44627700	-1.61038200	-2.87110900
C	-2.69133100	1.67054800	-0.30518800
C	-3.56894800	0.42822700	-0.14913900
O	-1.47148100	1.57188700	-0.09421100
C	-3.33218100	-1.89546600	0.35930900
C	-2.24295300	-2.94390700	0.65527400
O	-2.58991500	-4.09986400	0.81697100
O	-1.04073700	-2.45594100	0.69631300
O	-2.73039700	-0.59438000	0.31878100
H	-4.39067300	0.61333000	0.55929700
H	-4.01323100	0.15794600	-1.12070800
H	-3.79467600	-2.12308100	-0.61073600
H	-4.10460500	-1.92997200	1.13709900
O	0.11206700	-0.15148600	1.87211300
O	-0.28915000	-0.81463200	-1.51685200
N	3.20511600	2.31639900	0.94938500
C	4.64454000	2.44949500	1.14751300

H	4.97696100	1.84392400	2.00025800
H	5.20211200	2.14549100	0.26305600
H	4.88314500	3.49853600	1.35450800
C	2.37431100	2.95083500	1.97152700
H	1.33272500	2.69392900	1.79238500
H	2.67091300	2.59133800	2.96343500
H	2.50306000	4.03949300	1.93652200
N	-3.26050300	2.83639300	-0.67391300
C	-2.43078100	4.02867500	-0.84199300
H	-1.39060000	3.76430200	-0.66110900
H	-2.54063300	4.41488400	-1.86172500
H	-2.74430500	4.80535800	-0.13441100
C	-4.68449800	3.01784200	-0.92956600
H	-4.83229700	3.40773100	-1.94344700
H	-5.23121100	2.08011700	-0.84240100
H	-5.10948600	3.73611300	-0.21776000
Pu	-0.07055100	-0.49735100	0.17877300

2:1 Pu(VI)/ODA

C	-2.70576200	2.01343400	-0.46032000
C	-3.71669500	0.91160400	-0.07144200
O	-1.46329700	1.68958500	-0.38755200
C	-3.48448400	-1.22290000	0.95781300
C	-2.64710900	-1.96547800	-0.11581600
O	-3.02007700	-3.10486700	-0.40632800
O	-1.63675200	-1.33665400	-0.61316500
O	-3.28973300	0.16842400	1.05430200
H	-4.68484700	1.39347700	0.13251700
H	-3.83936800	0.25866800	-0.94869100
H	-4.54361300	-1.48030500	0.78453200
H	-3.20078500	-1.63356300	1.93418300
O	-0.26222000	-0.07969200	1.68855200
O	0.55524100	0.16209000	-1.69826900
Pu	0.11668600	0.05054800	-0.00863100
O	-3.16173900	3.08928000	-0.86101700
C	2.37888900	-2.45975500	-0.07152200
C	3.39524900	-1.31163800	-0.24136800
O	1.17938800	-2.07290000	0.16119000
C	3.52321100	1.07357700	-0.05026100
C	2.63344100	2.28112400	0.30987100
O	3.17862500	3.38744300	0.37524800
O	1.39835200	1.99180800	0.49195800
O	2.82467900	-0.11730200	0.25657800

H	4.32686100	-1.55604300	0.29109200
H	3.63450400	-1.20172500	-1.31256500
H	3.75757300	1.11076400	-1.12750600
H	4.47150700	1.12942400	0.50543500
O	2.80368900	-3.61372100	-0.18517300

4. The coordinates of the optimized structures of U(VI) complexes by DFT methods.

U(VI)/5H₂O

O	1.74763500	-1.76531800	-0.00028500
O	-0.38284700	2.45428200	0.00101200
O	2.21777500	1.11993800	-0.00022200
O	0.00042900	-0.00009100	1.74670200
O	0.00269400	0.00009600	-1.74654800
O	-2.45182600	0.39736000	-0.00230500
H	-2.98224700	0.74362800	-0.74366900
H	-3.06458000	0.24102700	0.73998000
O	-1.13958000	-2.20739000	0.00077500
H	-1.62974000	-2.60575700	-0.74216200
H	-1.17949300	-2.83966300	0.74206900
H	1.98073000	-2.34815100	-0.74655100
H	2.84615100	1.15969400	-0.74487000
H	-0.22180700	3.06704500	-0.74027400
H	2.62567200	1.59907700	0.74474600
H	-0.71487900	2.98788800	0.74664700
H	2.33091500	-2.00516000	0.74348900
U	0.00059800	0.00010200	0.00008200

1:1 U(VI)/TMOGA-H₂O

Title Card Required

O	1.58225600	-2.92527500	0.00043600
O	-1.58218700	-2.92530200	0.00023000
C	2.35264500	1.37204000	-0.00014500
C	1.19857600	2.37269700	0.00044500
O	2.04319100	0.14094500	-0.00030900
C	-1.19859700	2.37269100	0.00051200
C	-2.35265800	1.37202600	0.00012600
O	-2.04319400	0.14093400	-0.00001900
O	-0.00000800	1.59358800	0.00010000
H	1.22948200	3.00842700	0.89454300

H	1.22937500	3.00941100	-0.89294700
H	-1.22949300	3.00933000	-0.89293000
H	-1.22941200	3.00849500	0.89456000
O	0.00011100	-1.08864300	1.75583100
O	-0.00012400	-1.08910700	-1.75564800
N	3.60409800	1.79314100	-0.00048900
C	4.72650000	0.83795200	-0.00129100
H	4.34343100	-0.17936100	-0.00337500
H	5.33781400	1.00780900	-0.89219700
H	5.33658000	1.00465500	0.89106700
C	3.99886200	3.21086400	-0.00025400
H	4.59873700	3.41620500	-0.89169600
H	3.13466800	3.87333700	0.00238600
H	4.60268400	3.41460300	0.88887000
N	-3.60411400	1.79311700	-0.00005500
C	-3.99888800	3.21083700	0.00012500
H	-3.13469700	3.87331700	0.00235900
H	-4.59906900	3.41604300	-0.89114100
H	-4.60240700	3.41470300	0.88942700
C	-4.72650800	0.83791900	-0.00062100
H	-5.33775000	1.00744100	-0.89164200
H	-4.34343200	-0.17939100	-0.00229000
H	-5.33666400	1.00494900	0.89162400
H	1.97821700	-3.34246100	0.78586700
H	1.97797900	-3.34308800	-0.78478200
H	-1.97793600	-3.34291900	0.78553900
H	-1.97795500	-3.34283700	-0.78511300
U	0.00000000	-1.01241000	0.00008000

1:1 U(VI)/DMOGA-H₂O

C	2.54069100	0.17188400	-0.00079500
C	2.10210600	1.63598600	-0.00026800
O	1.63920500	-0.70887600	-0.00170300
C	0.05719100	2.92232000	0.00049400
C	-1.46419300	2.71759100	-0.00018800
O	-2.21085000	3.66440000	0.00078600
O	-1.80986300	1.43892300	-0.00210700
O	0.68625000	1.62439500	-0.00106900
H	2.47706200	2.15565500	0.89221400
H	2.47797100	2.15673000	-0.89173400
H	0.35587100	3.48281800	-0.89265800
H	0.35534400	3.48035700	0.89537100
O	-0.77609200	-0.60638300	1.76531900

O	-0.77856100	-0.61053500	-1.76530800
N	3.83461400	-0.13572200	-0.00033600
C	4.27064200	-1.53850500	-0.00022800
H	3.39985600	-2.18982000	-0.00084300
H	4.87679700	-1.72910900	-0.89134400
H	4.87571200	-1.72933300	0.89158700
C	4.91730200	0.85313900	0.00137400
H	5.54210300	0.71036800	-0.88604500
H	4.53452600	1.87234900	-0.00261000
H	5.53599600	0.71464400	0.89378200
O	-0.67247100	-3.00733800	0.00216000
H	-0.84220800	-3.55585400	-0.78181400
H	-0.84143000	-3.55477800	0.78704900
O	-3.21638900	-1.11430500	0.00182200
H	-3.68402400	-0.75397900	-0.77345600
H	-3.68369300	-0.75033800	0.77555700
U	-0.75711400	-0.49322200	-0.00015500

1:1 U(VI)/ODA-H₂O

C	-2.40498700	1.62326100	-0.02024300
C	-1.21877900	2.59992900	-0.04984100
O	-2.04581000	0.35687300	-0.01787100
C	1.21922300	2.59976000	-0.04983900
C	2.40525800	1.62289100	-0.02035000
O	3.53986800	2.05081700	0.00127100
O	2.04586600	0.35656000	-0.01816000
O	0.00017200	1.85097900	-0.12468700
H	-1.30647900	3.26330200	-0.91836000
H	-1.22700200	3.20973900	0.86229400
H	1.22757600	3.20951700	0.86233000
H	1.30700200	3.26316400	-0.91832800
O	-0.00018500	-0.89313500	-1.73704700
O	0.00005700	-0.59900000	1.79395400
O	-3.53952800	2.05138000	0.00126200
O	1.93736800	-2.35155100	0.04860900
H	2.61226700	-1.66448000	0.23518200
H	2.13860700	-2.65439800	-0.85333700
O	-1.93773500	-2.35129300	0.04846200
H	-2.13889900	-2.65383500	-0.85360500
H	-2.61255800	-1.66417900	0.23513800
U	-0.00005800	-0.63866200	0.02417400

2:1 U(VI)/TMOGA

C	-2.32659900	2.54870400	0.03334100
C	-1.18851500	3.52024900	-0.25856600
O	-2.03174900	1.33770500	0.19040600
C	1.18840800	3.52026600	-0.25867700
C	2.32653100	2.54876600	0.03323200
O	2.03173000	1.33775600	0.19031000
O	-0.00004200	2.76025400	-0.11268200
H	-1.26771900	3.92254100	-1.27878700
H	-1.19252300	4.35800700	0.45099900
H	1.19243400	4.35807300	0.45082800
H	1.26755000	3.92248900	-1.27893000
O	-0.00001600	0.13411400	-1.75322000
O	0.00001800	-0.13415400	1.75321300
N	-3.57387700	3.00373100	0.12153300
C	-4.67607700	2.09531100	0.46112900
H	-4.26966600	1.12595400	0.74153500
H	-5.23929500	2.51633100	1.29930600
H	-5.34484100	1.98837400	-0.39931500
C	-3.95327300	4.40854300	-0.07169500
H	-4.21515000	4.86594300	0.88845100
H	-3.15256200	4.98177700	-0.53770800
H	-4.82513600	4.45030900	-0.73047700
N	3.57379900	3.00383500	0.12134200
C	3.95312300	4.40866100	-0.07192800
H	3.15245800	4.98178900	-0.53815300
H	4.21478900	4.86616900	0.88822500
H	4.82510300	4.45043300	-0.73055100
C	4.67604400	2.09547100	0.46094300
H	5.23920500	2.51649000	1.29916100
H	4.26968300	1.12607800	0.74129500
H	5.34484700	1.98861400	-0.39948000
C	-2.32654200	-2.54876200	-0.03329800
C	-1.18842400	-3.52030200	0.25851400
O	-2.03170100	-1.33775600	-0.19034000
C	1.18849800	-3.52026500	0.25859000
C	2.32660000	-2.54871700	-0.03325400
O	2.03175700	-1.33771100	-0.19028100
O	0.00002900	-2.76028900	0.11254800
H	-1.26755300	-3.92259300	1.27874100
H	-1.19246600	-4.35805800	-0.45105200
H	1.19257400	-4.35806400	-0.45092000
H	1.26761000	-3.92248900	1.27884600
N	-3.57381200	-3.00379600	-0.12152800

C	-4.67601900	-2.09536000	-0.46105100
H	-4.26961900	-1.12596500	-0.74133900
H	-5.23921100	-2.51629800	-1.29928900
H	-5.34480700	-1.98853400	0.39938800
C	-3.95321300	-4.40860900	0.07168400
H	-4.21529900	-4.86593100	-0.88844100
H	-3.15242400	-4.98190400	0.53748600
H	-4.82494400	-4.45039500	0.73063900
N	3.57388800	-3.00373000	-0.12137400
C	3.95331000	-4.40851800	0.07196100
H	3.15249800	-4.98180500	0.53773200
H	4.21548700	-4.86589100	-0.88811600
H	4.82498900	-4.45024500	0.73099100
C	4.67610400	-2.09529000	-0.46085500
H	5.23931800	-2.51621400	-1.29908500
H	4.26971300	-1.12589100	-0.74114000
H	5.34487000	-1.98847700	0.39960300
U	0.00000200	-0.00001200	-0.00000300

2:1 U(VI)/DMOGA-trans

O	0.68051300	4.37858300	-0.01450100
C	0.08381700	3.32365800	-0.15297300
C	-1.44106000	3.29713500	0.05906200
O	-1.92381400	2.02026100	-0.35722400
C	-3.22844000	1.69066700	0.04275000
C	-3.36841500	0.19491900	-0.25613000
N	-4.53146300	-0.43950000	-0.03307400
O	0.59459600	2.16754500	-0.46278400
O	-2.37014600	-0.41073200	-0.68509000
C	-4.60421800	-1.89036900	-0.23869500
C	-5.76075000	0.21826700	0.39028400
H	-1.65378800	3.45504000	1.12587200
H	-1.91481700	4.09945800	-0.51942800
H	-3.37281700	1.87404700	1.11929400
H	-3.97305000	2.28223700	-0.51092900
H	-5.18026800	-2.33277600	0.57984500
H	-5.10149200	-2.11927000	-1.18886100
H	-3.59644000	-2.30523600	-0.24377600
H	-5.61301200	1.28929900	0.52559100
H	-6.10453500	-0.20655500	1.34043700
H	-6.54677500	0.06926600	-0.36007200
O	-0.68051000	-4.37858300	0.01449100
C	-0.08381100	-3.32366000	0.15297000
C	1.44106400	-3.29713700	-0.05907600

O	1.92382200	-2.02026800	0.35722200
C	3.22844200	-1.69066500	-0.04276400
C	3.36841300	-0.19491800	0.25612600
N	4.53145400	0.43951100	0.03305800
O	-0.59458700	-2.16755000	0.46279700
O	2.37014700	0.41072300	0.68510500
C	4.60419800	1.89037900	0.23868600
C	5.76074100	-0.21824300	-0.39032100
H	1.91482500	-4.09946700	0.51940000
H	1.65378300	-3.45502800	-1.12589100
H	3.97306100	-2.28223700	0.51090100
H	3.37280800	-1.87403500	-1.11931100
H	3.59641800	2.30523900	0.24376700
H	5.10147100	2.11928000	1.18885300
H	5.18024700	2.33279300	-0.57985300
H	5.61301300	-1.28927600	-0.52562700
H	6.54677700	-0.06923500	0.36002200
H	6.10450700	0.20658400	-1.34047900
O	0.50541000	-0.43086000	-1.64959100
O	-0.50540800	0.43085600	1.64960300
U	0.00000100	-0.00000200	0.00000700

2:1 U(VI)/ODA

C	2.73635100	-2.01269300	-0.43964500
C	3.75541300	-0.92539600	-0.03213200
O	1.49527500	-1.68351600	-0.33729500
C	3.53902000	1.21214000	0.99229600
C	2.70641700	1.96149900	-0.08039300
O	3.09590300	3.08953400	-0.38903900
O	1.67492500	1.34289100	-0.54725100
O	3.32613600	-0.17715200	1.08935400
H	4.71533700	-1.41956100	0.18100000
H	3.89782400	-0.27329400	-0.90730100
H	4.60098400	1.45562500	0.81748400
H	3.26143600	1.62659100	1.96891100
O	0.16389700	0.09614300	1.72221600
O	-0.53891800	-0.16199200	-1.76945800
O	3.18317100	-3.07704500	-0.87519900
C	-2.41316700	2.47043600	-0.08215400
C	-3.43574200	1.31774000	-0.16122200
O	-1.19703600	2.09157600	0.06141500
C	-3.56150500	-1.06778400	0.03812500
C	-2.66371400	-2.29124600	0.31582400

O	-3.22116900	-3.38866200	0.40818800
O	-1.41344700	-2.02218500	0.40450500
O	-2.81432800	0.11508100	0.25213100
H	-4.30491700	1.54644500	0.47363400
H	-3.79010900	1.22395200	-1.20119600
H	-3.91328100	-1.11106800	-1.00607400
H	-4.44426300	-1.09649100	0.69444100
O	-2.85380800	3.61943600	-0.17800600
U	-0.12180700	-0.05101400	-0.03323500

5. The coordinates of the optimized structures of Np(V) complexes by DFT methods.

Np(V)/5H₂O

O	-0.79875200	2.44266200	-0.00188100
O	-0.77785600	-2.44943000	0.00010100
O	-2.57033900	-0.01223900	-0.00180900
O	-0.00169000	0.00229000	1.78832400
O	-0.00228100	-0.00095100	-1.78718600
O	2.08551000	-1.49865700	-0.00270300
H	2.40199600	-2.03786100	-0.74360300
H	2.69233400	-1.63797800	0.74040500
O	2.07727200	1.51210000	0.00012900
H	2.67693600	1.65713100	-0.74771800
H	2.39233900	2.05743200	0.73714800
H	-0.75823100	3.05579600	-0.75178500
H	-3.14230000	0.22829600	-0.74674400
H	-1.19133100	-2.91828400	-0.74091400
H	-3.14443000	-0.24340900	0.74444300
H	-0.73365600	-3.06553800	0.74734800
H	-1.20764800	2.91469500	0.73966400
Np	-0.00087000	0.00025300	0.00066600

1:1 Np(V)/TMOGA-2H₂O

O	1.70337700	2.99662400	0.00035100
O	-1.70302600	2.99687100	0.00055600
C	2.37444900	-1.40722100	-0.00005000
C	1.18192100	-2.37038300	0.00018200
O	2.16535700	-0.18040400	-0.00027600
C	-1.18200800	-2.37035800	-0.00031800

C	-2.37451700	-1.40716700	-0.00041400
O	-2.16538900	-0.18035900	-0.00025500
O	-0.00003500	-1.58982100	-0.00025900
H	1.20943600	-3.01364700	-0.89116000
H	1.20920300	-3.01299900	0.89200900
H	-1.20949400	-3.01331000	0.89126000
H	-1.20933800	-3.01328300	-0.89191000
O	-0.00007200	1.13783300	-1.79417200
O	0.00011700	1.13714300	1.79430100
N	3.61239200	-1.92976000	0.00017000
C	4.78120800	-1.04641800	-0.00020200
H	4.44737200	-0.01144100	-0.00138100
H	5.38785900	-1.23740300	0.89152000
H	5.38855200	-1.23920400	-0.89105800
C	3.91817600	-3.35942100	0.00051400
H	4.50735700	-3.61204600	0.88906400
H	3.01574300	-3.96871300	0.00219400
H	4.50495900	-3.61314400	-0.88932500
N	-3.61247900	-1.92966300	-0.00032500
C	-3.91832500	-3.35931100	-0.00049800
H	-3.01592200	-3.96864700	-0.00071600
H	-4.50621700	-3.61261300	0.88872100
H	-4.50642300	-3.61230400	-0.88967000
C	-4.78125500	-1.04626800	-0.00027400
H	-5.38891200	-1.23913400	0.89034700
H	-4.44737100	-0.01130600	0.00112300
H	-5.38760800	-1.23711900	-0.89223100
H	2.23042400	3.22211900	-0.78201100
H	2.23053900	3.22164200	0.78277300
H	-2.22993800	3.22271600	-0.78179500
H	-2.22992800	3.22239700	0.78300600
Np	-0.00000200	1.08816800	0.00005100

1:1 Np(V)/DMOGA-2H₂O

C	-2.58180500	0.16314900	-0.05647000
C	-2.07855600	1.60328300	0.08021600
O	-1.76886100	-0.76678800	-0.18424600
C	-0.05964300	2.87438100	0.07924200
C	1.47815700	2.74375300	0.02419000
O	2.11688300	3.78203200	0.11273800
O	1.92237400	1.53724700	-0.10086100
O	-0.69402800	1.60164500	-0.14550300

H	-2.58623800	2.25964200	-0.64270000
H	-2.30728000	1.97644100	1.09237900
H	-0.34440700	3.25282800	1.07027600
H	-0.39443000	3.59107600	-0.68056300
O	0.93226800	-0.79537600	-1.80115600
O	0.58359500	-0.50206200	1.77148500
N	-3.91661900	-0.05089700	-0.02533900
C	-4.44328100	-1.40158000	-0.20538600
H	-3.61389300	-2.08453400	-0.37709500
H	-4.99749800	-1.71220300	0.68809000
H	-5.12119200	-1.42499800	-1.06670700
C	-4.91720000	1.00088400	0.11981300
H	-5.67515300	0.67632300	0.84077000
H	-4.47752700	1.92465900	0.49375600
H	-5.41543200	1.20566800	-0.83662900
O	0.81792600	-3.11161700	0.47035400
H	0.56073000	-3.20437500	1.40179800
O	3.38923300	-0.62953400	-0.01214700
H	3.60072600	-0.80465200	-0.94410100
Np	0.77127300	-0.56665300	-0.02155900
H	0.33545000	-3.78424900	-0.03356800
H	3.34292600	0.35580500	0.04168500

1:1 Np(V)/ODA-2H₂O

C	-2.43501700	1.65182400	-0.09926700
C	-1.20187700	2.57760900	-0.03180400
O	-2.16749600	0.39024900	-0.16765100
C	1.20208900	2.57754000	-0.03184300
C	2.43516700	1.65165900	-0.09919500
O	3.54082300	2.18449400	-0.06396300
O	2.16755800	0.39009200	-0.16725400
O	0.00007900	1.85894400	-0.30063500
H	-1.32290400	3.39738400	-0.75270100
H	-1.15441400	3.01495000	0.97703200
H	1.15463700	3.01496300	0.97695900
H	1.32318400	3.39724600	-0.75280300
O	0.00010900	-1.22032100	-1.66412800
O	-0.00018900	-0.35261700	1.85071700
O	-3.54063500	2.18471800	-0.06382500
O	2.21514400	-2.22989200	0.01058700
H	2.65942800	-1.34618900	0.03668900
H	2.06235700	-2.36346200	-0.94119100
O	-2.21528500	-2.22972600	0.01053100

H	-2.06259100	-2.36334500	-0.94125400
H	-2.65947900	-1.34597600	0.03663800
Np	-0.00003500	-0.68779400	0.07933600

1:2 Np(V)/TMOGA

C	-2.34655800	2.55128700	0.16186300
C	-1.17810700	3.46428300	-0.21614000
O	-2.11265300	1.37772100	0.48699200
C	1.17776300	3.46437100	-0.21611900
C	2.34627700	2.55148800	0.16195500
O	2.11245800	1.37792800	0.48717300
O	-0.00015100	2.80625400	0.20169200
H	-1.16998600	3.61805200	-1.30683300
H	-1.25841500	4.44422300	0.27383300
H	1.25797700	4.44433300	0.27382800
H	1.16966400	3.61810700	-1.30681700
O	0.00002000	0.53927100	-1.71299100
O	-0.00002800	-0.53927100	1.71300200
N	-3.59499100	3.05935000	0.11760900
C	-4.72973600	2.23075100	0.52375400
H	-4.35829300	1.26158100	0.85094600
H	-5.26687400	2.71596600	1.34661400
H	-5.41827200	2.09982900	-0.31882400
C	-3.91455900	4.43254200	-0.26477300
H	-4.11310700	5.05497900	0.61690900
H	-3.11208000	4.88401000	-0.84823600
H	-4.81214300	4.42479600	-0.89070900
N	3.59466800	3.05965600	0.11770300
C	3.91412700	4.43284600	-0.26477400
H	3.11160700	4.88421300	-0.84825700
H	4.11263600	5.05535500	0.61686600
H	4.81170500	4.42512700	-0.89071900
C	4.72947700	2.23117700	0.52391600
H	5.26666100	2.71658200	1.34663300
H	4.35810000	1.26205800	0.85133100
H	5.41795100	2.10011100	-0.31869100
C	-2.34627700	-2.55151700	-0.16189300
C	-1.17773200	-3.46440100	0.21608800
O	-2.11249600	-1.37793100	-0.48704500
C	1.17813300	-3.46427100	0.21605300
C	2.34656100	-2.55124300	-0.16193300
O	2.11263100	-1.37768500	-0.48708400
O	0.00015800	-2.80626400	-0.20175900

H	-1.16957700	-3.61816800	1.30678100
H	-1.25795900	-4.44434800	-0.27388500
H	1.25846900	-4.44420200	-0.27393700
H	1.17001900	-3.61805900	1.30674300
N	-3.59465800	-3.05970500	-0.11760700
C	-4.72949800	-2.23122000	-0.52372000
H	-4.35816100	-1.26202600	-0.85095900
H	-5.26663100	-2.71651100	-1.34653900
H	-5.41800500	-2.10033700	0.31888700
C	-3.91408100	-4.43292200	0.26480200
H	-4.11266900	-5.05536600	-0.61686600
H	-3.11150700	-4.88433100	0.84817700
H	-4.81160300	-4.42525100	0.89082900
N	3.59500000	-3.05929000	-0.11768800
C	3.91458400	-4.43247900	0.26468500
H	3.11206100	-4.88399600	0.84804900
H	4.11324300	-5.05487800	-0.61699900
H	4.81210500	-4.42472000	0.89071200
C	4.72974000	-2.23067400	-0.52381600
H	5.26693700	-2.71592200	-1.34661800
H	4.35828600	-1.26153400	-0.85108200
H	5.41822700	-2.09968200	0.31879200
Np	-0.00000700	-0.00000400	0.00000400

1:2 Np(V)/DMOGA-trans

O	-0.87455100	4.51464000	-0.08813300
C	-0.32969700	3.41854800	0.07772400
C	1.21577300	3.40603500	-0.02348000
O	1.74892600	2.22176300	0.57113500
C	3.01220900	1.83529300	0.10280500
C	3.18002000	0.35922500	0.48914000
N	4.26151000	-0.32732200	0.05182100
O	-0.88140300	2.28255500	0.28190900
O	2.30779700	-0.18978600	1.17341500
C	4.27278600	-1.78366400	0.23570700
C	5.34592600	0.25901300	-0.71430000
H	1.48076500	3.43630700	-1.09085500
H	1.62767700	4.29902800	0.46504900
H	3.06698300	1.93033000	-0.99113800
H	3.81437100	2.45100800	0.54832400
H	4.84545700	-2.22858700	-0.58419600
H	4.74543100	-2.05790800	1.18783500
H	3.24756800	-2.16403300	0.20931200

H	5.30243700	1.34848600	-0.68569300
H	5.31048700	-0.06321100	-1.76409200
H	6.31122700	-0.04962100	-0.29239700
O	0.87458000	-4.51461300	0.08823600
C	0.32968800	-3.41854900	-0.07768600
C	-1.21577500	-3.40605000	0.02363000
O	-1.74897500	-2.22185100	-0.57108200
C	-3.01222600	-1.83532800	-0.10271300
C	-3.18001900	-0.35926700	-0.48909100
N	-4.26148400	0.32731500	-0.05176200
O	0.88135100	-2.28256200	-0.28201500
O	-2.30782300	0.18970600	-1.17343000
C	-4.27276700	1.78364400	-0.23575700
C	-5.34591300	-0.25896200	0.71438100
H	-1.62770900	-4.29910600	-0.46475700
H	-1.48068000	-3.43619100	1.09103200
H	-3.81442700	-2.45102800	-0.54818500
H	-3.06696200	-1.93033400	0.99123400
H	-3.24755600	2.16403100	-0.20934100
H	-4.74536900	2.05781200	-1.18792800
H	-4.84548600	2.22861800	0.58408400
H	-5.30230000	-1.34843600	0.68603400
H	-6.31121600	0.04947000	0.29232900
H	-5.31059800	0.06350400	1.76410200
O	-0.86588200	-0.41996000	1.53773600
O	0.86588100	0.41999200	-1.53780800
Np	0.00000500	0.00001300	-0.00003300

1:2 Np(V)/ODA

O	0.45005900	-0.00020000	-1.76448500
O	-0.45040000	0.00004300	1.76383200
C	-2.62699500	-2.40580200	-0.15528000
C	-3.47501300	-1.18951300	0.29560900
O	-1.42232900	-2.14412300	-0.43736300
C	-3.47490800	1.18988800	0.29540400
C	-2.62686600	2.40599300	-0.15587500
O	-3.22455700	3.50562600	-0.16855700
O	-1.42206300	2.14428500	-0.43737000
O	-2.88935000	0.00011700	-0.18403600
H	-4.50936100	-1.29908600	-0.07739000
H	-3.51911600	-1.17169500	1.40028600
H	-3.51885600	1.17231600	1.40009400

H	-4.50928900	1.29942100	-0.07750000
O	-3.22461100	-3.50547900	-0.16711900
Np	-0.00013200	-0.00004900	-0.00032000
C	2.62700900	-2.40595500	0.15576200
C	3.47532600	-1.18971500	-0.29472700
O	1.42213300	-2.14421200	0.43685100
C	3.47559100	1.18968300	-0.29418400
C	2.62727600	2.40589400	0.15638500
O	3.22504700	3.50548300	0.16936800
O	1.42228000	2.14423300	0.43697500
O	2.88918800	-0.00006000	0.18425700
H	4.50940500	-1.29911400	0.07906300
H	3.52029500	-1.17209600	-1.39938800
H	3.52093300	1.17239300	-1.39883800
H	4.50956200	1.29885700	0.07996500
O	3.22462200	-3.50562100	0.16826700