

Electronic Supplementary Information for

A computational study on the coordination modes and electron absorption spectra of the complexes U(IV) with N, N, N', N'-tetramethyl-diglycolamide and anions

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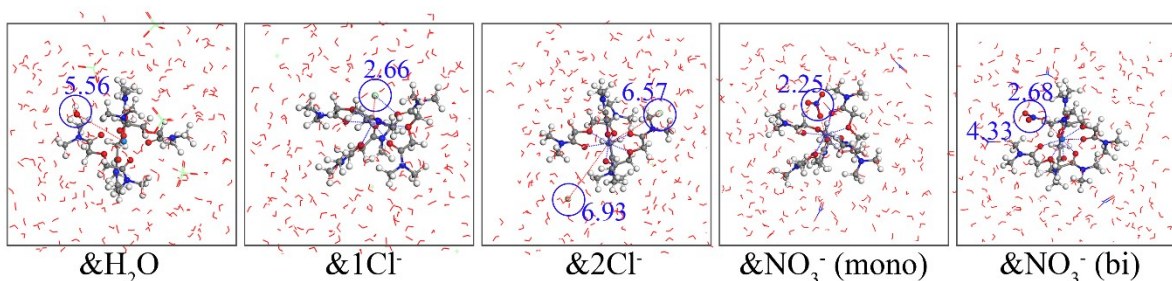


Figure S1. Snapshot of geometry for U(IV)-TMDGA complexes with and without water and counterions Cl⁻, NO₃⁻ during AIMD after 1 ps. The water cube contains more than 200 water molecules with cubic parameters at 20 Å to mimic the real solvent condition, also, the counterions are replenished to keep electroneutrality. The red, white, blue, dark blue and green ball represents oxygen, hydrogen, uranium, nitrogen and chloride atoms. The distance of U-Cl in &2Cl⁻ system is far away from the maximum limit for coordination, as well as the U-O(H₂O) distance in &H₂O system.

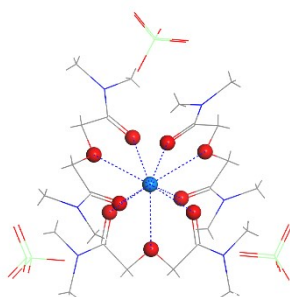


Figure S2. Geometric schematic diagram of non-ligand U(IV)-TMDGA complexes, with 3 perchlorate ions (ClO₄⁻) symmetrically introduced in non-ligand U(IV)-TMDGA complex in the outer coordination sphere to mimic the real condition. The red and blue ball represents the oxygen and uranium atom, and the green dot is for chloride. Three ClO₄⁻s are placed in three corners.

Table S1. Comparison of calculated (Calc.) and experimental (Exp.) absorption spectra¹ of U(IV)-TMDGA complexes with and without counterions, as well as the assignment of excited states. TMDGA represents the pure U(IV)-TMDGA complex, the &Cl⁻, &NO₃⁻(mono) and &NO₃⁻(bi) represents TMDGA-U(IV) complexes with counterions.

Spectral Branches	Degeneracy	peak	Wavelength (nm)					Excited states
			Exp. ¹		Calc.			
			&NO ₃ ⁻	TMDGA	&Cl ⁻	&NO ₃ ⁻ (mono)	&NO ₃ ⁻ (bi)	
³ H ₄	9			∞	∞	∞	∞	0-8
³ F ₂	5			5000.0				9-13
				4400.0	5400.7	4873.7	5327.0	4806.5
³ H ₅	11			2288.6	2555.3	2459.3	2376.9	14-24
					2236.7	2143.5	2242.7	
³ F ₃ ³ F ₄	16			1440.3	1442.6	1422.6	1397.5	25-40
				1350.8	1326.2	1364.1	1351.5	
				1107.5	1152.4		1103.6	41-53
				1065.8	1088.0	1143.2	1030.1	
³ H ₆	13			998.8	1000.3		983.5	
				964.9	973.4	1086.9	933.5	
				916.6	946.1	917.5	905.9	
					715.8	695.2	700.9	54-68
³ P ₀ ¹ D ₂ ¹ G ₄	15	a/a ₀	670.0					
		b/b ₀	659.3	709.8	696.1	672.9	685.7	
		c/c ₀	653.0	695.2	679.3	661.5	672.9	
		d/d ₀	625.8		661.5	650.4	658.9	
³ P ₁	3	e/e ₀	551.3	561.4	567.8	554.7	559.0	69-71
		f/f ₀	541.0	551.6	551.0	541.6	541.0	
¹ I ₆	13	g/g ₀	491.5	491.5	473.5	479.8	478.5	72-84
		h/h ₀	477.3	477.1	454.4	471.8	469.1	
		i/i ₀	465.8	467.4	444.4	447.9	445.9	
³ P ₂	5	j/j ₀	432.5	442.4	429.3	426.0	418.2	85-89
		k/k ₀	418.0	402.2	416.2	407.4	400.6	
¹ S ₀	1			356.3	225.4	225.0	224.3	90

References

- [1] Q. Liu, J. Zhou, L. Zhu, D. Li, Y. Zhang, S. Yang and G. Tian, The complexation of U(IV) ion with N, N', N'-Tetraalkyl-Diglycolamide in aqueous solutions and extraction systems of varying anions, *Inorg. Chem. Commun.*, 2022, **143**: 109730.

Optimized geometries for U(IV)-TMDGA Complexes in xyz format. The units of coordinates are angstrom(Å).

1. U(IV)-TMDGA

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TMDGA

C	0.12446900	3.21050600	3.72010600
H	0.12179400	2.71390300	4.69576600
H	0.93375600	2.82142500	3.10996600
H	0.25788400	4.28421000	3.87876400
C	-2.30372500	3.76097700	3.54114300
H	-2.25209100	4.79089500	3.17217800
H	-3.25155400	3.31240300	3.24540900
H	-2.27083000	3.78324100	4.63323600
C	-1.22389600	2.19015300	2.02620800
C	-2.52084100	1.98470200	1.30721800
H	-2.93313000	2.93569400	0.94480200
H	-3.26849600	1.51275500	1.95952800
C	-3.33151800	0.90937700	-0.63997700
H	-4.18323900	0.54203500	-0.05302600
H	-3.62582400	1.85035600	-1.12353600
C	-2.88135500	-0.10588700	-1.64778000
C	-5.13327600	-0.14952600	-2.59259200
H	-5.33014900	0.73712100	-1.99200200
H	-5.41420200	0.07662300	-3.62482900
H	-5.76298400	-0.97317000	-2.23880500
C	-3.31866300	-1.51304700	-3.55615700
H	-2.25895900	-1.73121600	-3.45248400
H	-3.90424300	-2.43106700	-3.43943800
H	-3.51122600	-1.10843900	-4.55447700
C	-2.71279100	-2.17497000	3.62593800
H	-2.47931500	-2.56940900	4.61902800
H	-2.33390300	-1.15957600	3.54022400
H	-3.79995100	-2.18598800	3.49679900
C	-2.25653300	-4.47068600	2.79371700
H	-3.28498400	-4.66706900	3.10681000
H	-2.08028500	-5.01879400	1.86915500
H	-1.58165700	-4.83892000	3.57384400
C	-1.37130400	-2.50397200	1.65427300
C	-0.68414400	-3.41018900	0.67321100
H	-1.40038600	-4.01200600	0.09948000
H	0.01364600	-4.09018600	1.17831800
C	0.82244500	-3.26936200	-1.16664200
H	1.50861800	-3.94783900	-0.64420600
H	0.17216000	-3.87027900	-1.81685800
C	1.57242100	-2.23060400	-1.94882500
C	2.82531300	-4.04864900	-3.01325000
H	3.17921600	-4.16500200	-4.03924200
H	1.95796600	-4.69677400	-2.88595900
H	3.62635900	-4.34895800	-2.32980100
C	3.30957700	-1.63867600	-3.49686800

H	3.01245100	-0.63468300	-3.20753100
H	4.35907700	-1.81435900	-3.24042300
H	3.19128300	-1.75851400	-4.57763800
C	3.30322300	-1.53210100	3.36762100
H	3.63540800	-1.30080600	4.38270100
H	2.22395800	-1.66415400	3.35751200
H	3.79979900	-2.45119500	3.03926200
C	5.01974400	0.15996200	2.67227400
H	5.71731300	-0.64684000	2.91031100
H	5.37586800	0.65415300	1.76973900
H	5.01273100	0.86896300	3.50650200
C	2.87286400	-0.03702100	1.52805900
C	3.26567800	1.10378700	0.64093500
H	4.11683500	0.84249600	-0.00275000
H	3.54151100	1.98718200	1.23057600
C	2.23102200	2.61348000	-0.88253500
H	2.31533700	3.45432800	-0.18178800
H	3.12514600	2.59233600	-1.51693100
C	0.96188800	2.70663100	-1.70178100
C	1.79045900	4.74871900	-2.76577000
H	2.14475300	4.69021000	-3.79959200
H	1.32139700	5.72519200	-2.61401700
H	2.64334200	4.66964500	-2.09371900
C	-0.48679400	3.87144700	-3.23773900
H	-1.05960300	4.66762800	-2.75175500
H	-0.28105500	4.16611700	-4.26945500
H	-1.04258800	2.93768200	-3.22887100
N	-1.15952000	2.98940700	3.05226600
N	-3.73062300	-0.54271900	-2.55869000
N	-2.08737300	-3.02662300	2.61858500
N	2.47528900	-2.62682200	-2.80313500
N	3.67846300	-0.42262300	2.48822500
N	0.79855500	3.69683800	-2.53031600
O	-0.19469000	1.56072300	1.61854900
O	-2.21764500	1.13427100	0.21689000
O	-1.67539700	-0.50119100	-1.60117400
O	-1.20203900	-1.25685800	1.51543700
O	0.03750100	-2.54969500	-0.22119800
O	1.32080800	-1.01745100	-1.73556200
O	1.74690200	-0.59751000	1.33136300
O	2.12243300	1.38415500	-0.15890900
O	0.08434800	1.80558700	-1.54473500
U	0.00821900	-0.01902300	-0.06825400

2. H₂O-U(IV)-TMDGA

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TMDGA&H₂O

C	7.31599600	13.52628800	15.43405900
H	7.19825400	12.76255300	16.20722800
H	7.51242400	13.05423800	14.46943100
H	8.14627000	14.18748800	15.70748000

C	5.58726500	14.83200800	16.66606600
H	6.41870600	15.35803200	17.14413400
H	4.75141600	15.52219700	16.55659700
H	5.28003100	14.00079500	17.31023500
C	5.43868100	14.49660300	14.19687100
C	4.11885000	15.26532800	14.14072500
H	4.25463400	16.30160300	14.47246600
H	3.34948600	14.78876000	14.76504300
C	2.48970100	15.95515300	12.50080200
H	1.66706700	15.46420300	13.04246900
H	2.56640600	16.99291000	12.83901600
C	2.26910200	15.87405300	10.99443700
C	0.23472300	17.28305000	11.21363500
H	0.37065700	17.18688000	12.28637500
H	0.31206600	18.33838000	10.93309500
H	-0.76919300	16.92624400	10.96322600
C	0.98608400	16.42971600	8.98805700
H	1.84063200	15.97127300	8.49063100
H	0.08218200	15.83776900	8.81364500
H	0.83370900	17.44050600	8.59774100
C	2.63899000	10.38328800	13.28744500
H	2.93058100	9.36371000	13.56087400
H	3.39797800	11.08319900	13.62780900
H	1.67507900	10.61110900	13.75049200
C	1.69087200	9.38373300	11.20203900
H	0.73360200	9.33293000	11.72938000
H	1.49078500	9.55947200	10.14198100
H	2.21435700	8.42738400	11.31835600
C	3.11875300	11.42485100	11.11707900
C	3.03785400	11.42993500	9.59762500
H	2.01052300	11.58399600	9.24618300
H	3.42052600	10.48537500	9.17770300
C	3.97577800	12.70155900	7.75906300
H	4.27556200	11.76472700	7.26295900
H	2.99076400	13.00522600	7.37850000
C	5.00060600	13.79373800	7.54252600
C	4.71442600	13.61974200	5.07788200
H	5.43867400	13.00814200	4.52926700
H	4.41345500	14.45987000	4.44358600
H	3.83349300	13.01616100	5.30204100
C	6.36080300	15.20256000	6.09413100
H	6.97825900	15.31815100	6.98215600
H	6.98486200	14.89281800	5.25188900
H	5.87443800	16.15438000	5.84196900
C	7.80526800	9.74184400	10.58109200
H	8.31191200	9.15207900	11.35133100
H	6.77607800	9.92967900	10.88144300
H	7.83090800	9.18639700	9.63796100
C	9.98847600	10.91209600	10.23473400
H	10.18817200	10.14997500	9.47563100
H	10.43777400	11.84757200	9.89980400

H	10.45472300	10.60119900	11.17478400
C	7.85411100	12.18139300	10.45891700
C	8.61833100	13.48194700	10.27955500
H	9.02194400	13.57044300	9.26096100
H	9.43767200	13.57749500	11.00653800
C	8.21689300	15.86385100	10.31675900
H	9.04608400	16.01819800	11.02180000
H	8.60920300	15.97365300	9.29302300
C	7.07553900	16.82721500	10.56432800
C	8.64770200	18.69386800	10.20826600
H	8.50877100	19.71055000	9.83726100
H	9.24983800	18.73327600	11.12255200
H	9.15295800	18.11238800	9.43026000
C	6.22725300	19.12759000	10.74281000
H	5.30508300	18.62258800	11.01619500
H	6.52442500	19.80295600	11.55305100
H	6.07165000	19.71969300	9.83638200
N	6.06112500	14.31123500	15.35319200
N	1.23357900	16.49376600	10.44413100
N	2.51374000	10.45700400	11.80487800
N	5.33324800	14.16698500	6.31298600
N	8.51655000	11.03017900	10.41411400
N	7.30535400	18.13133700	10.49494300
O	5.92437800	14.07205400	13.07212800
O	3.72203100	15.25087300	12.75581800
O	3.11978800	15.19947100	10.30359500
O	3.77781000	12.35787700	11.69827100
O	3.91231800	12.50645800	9.18773300
O	5.51845000	14.32634900	8.59556700
O	6.58729300	12.23875900	10.63540200
O	7.65843500	14.52828100	10.51865400
O	5.91150400	16.33761300	10.84758000
U	5.13506100	14.09592400	10.87345500
O	9.24446500	16.82947200	7.40237000
H	10.13313600	16.60908200	7.10824400
H	9.03180300	17.63374700	6.90649600

3. Cl-U(IV)-TMDGA

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TMDGA&Cl-

Cl	-0.16085400	-0.12425300	-2.75010500
C	1.01642800	3.26852900	3.79035400
H	0.57780100	3.45585500	4.77483700
H	1.25574600	2.21235500	3.68902000
H	1.92393500	3.87199400	3.68798900
C	-0.52841600	4.99907900	2.90293300
H	0.27425300	5.69291200	3.16514600
H	-0.98289800	5.34816000	1.97602500
H	-1.27505200	5.00954900	3.70417700
C	-0.29600000	2.80002100	1.79418900
C	-1.35407400	3.21307500	0.77320700

H	-0.95966800	3.98210700	0.09604000
H	-2.25284600	3.60184000	1.26653400
C	-2.79578200	2.16284600	-0.82826500
H	-3.63865100	2.61290300	-0.28866200
H	-2.53738600	2.80367600	-1.68073700
C	-3.12983200	0.74232100	-1.28210500
C	-5.02161800	1.61278300	-2.62440500
H	-4.81692600	2.56915700	-2.14543700
H	-4.88870800	1.72125700	-3.70532500
H	-6.06245300	1.34227600	-2.42298500
C	-4.44263700	-0.79608700	-2.63232900
H	-3.60478500	-1.45769700	-2.42465500
H	-5.35485000	-1.17883600	-2.16242700
H	-4.59969900	-0.73623400	-3.71245400
C	-3.27811200	-1.03482700	3.75401900
H	-3.19001500	-1.55095900	4.71454100
H	-2.51865400	-0.25955800	3.68134700
H	-4.27605400	-0.59097600	3.68223800
C	-3.93218900	-3.21314100	2.75791900
H	-4.95402600	-2.90874200	2.99893900
H	-3.95760900	-3.75910000	1.81530600
H	-3.56741500	-3.87296400	3.55220300
C	-2.19256100	-1.79842100	1.71372500
C	-1.98916000	-2.85317000	0.62728100
H	-2.86077400	-2.89665300	-0.03751000
H	-1.81959000	-3.84563200	1.06128400
C	-0.35519700	-3.39174200	-1.05431800
H	-0.30971400	-4.38691700	-0.59511400
H	-1.02774100	-3.42472200	-1.92001200
C	1.03789800	-2.90680400	-1.45686200
C	1.27906200	-4.86666800	-2.95274800
H	1.13274500	-4.71514000	-4.02679200
H	0.34510900	-5.21625100	-2.51556800
H	2.03971800	-5.63909400	-2.80591900
C	3.05344700	-3.14964900	-2.79861100
H	3.23733400	-2.14807300	-2.41758800
H	3.83202600	-3.83550500	-2.44923500
H	3.06066700	-3.13254700	-3.89212400
C	2.31228600	-2.40463300	3.82152800
H	2.67174200	-2.11513800	4.81330500
H	1.27216000	-2.10844600	3.70536400
H	2.40848400	-3.48984300	3.71460100
C	4.58420400	-1.87207100	2.97553800
H	4.80984400	-2.91732200	3.20257300
H	5.12744200	-1.60006400	2.07111800
H	4.92924900	-1.25116700	3.80909500
C	2.55926800	-1.03036000	1.82783800
C	3.44226000	-0.30235700	0.81659700
H	3.95615800	-1.02259900	0.16696800
H	4.19125200	0.32297600	1.31755800
C	3.21443900	1.36270500	-0.88846100

H	3.98045800	1.96708400	-0.38534800
H	3.69587500	0.76521000	-1.67378400
C	2.10950400	2.24472400	-1.46676100
C	3.76010400	3.40544900	-2.89755200
H	3.82733300	3.10462600	-3.94768100
H	3.96851000	4.47675200	-2.82391400
H	4.51468600	2.86872300	-2.32439100
C	1.34497200	3.95324500	-3.01986800
H	1.41121000	4.98832000	-2.66884700
H	1.48505100	3.93723000	-4.10384800
H	0.37355500	3.53102500	-2.77363200
N	0.04647700	3.65297000	2.75432300
N	-4.13998000	0.54848800	-2.12326900
N	-3.09197900	-2.00914200	2.66826700
N	1.73860500	-3.61311100	-2.33688100
N	3.13049600	-1.73196000	2.80182100
N	2.40253200	3.14471200	-2.39539100
O	0.21533000	1.65222200	1.68659600
O	-1.67996400	2.03199500	0.04993000
O	-2.41594100	-0.19207600	-0.83119700
O	-1.48356800	-0.75670200	1.66027300
O	-0.83091200	-2.44708900	-0.09587700
O	1.46120600	-1.84501700	-0.92426600
O	1.30857200	-0.93581800	1.70140000
O	2.56641300	0.51888100	0.05541900
O	0.93955800	2.06559500	-1.02434000
U	-0.01902900	0.00475800	-0.10579400

4. NO₃⁻-U(IV)-TMDGA (monodentate)

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TMDGA&NO₃⁻ (mono)

O	0.62434600	-0.16027400	-2.18088500
C	2.33885600	-0.46943600	4.53925100
H	2.16574100	-0.06177400	5.53950300
H	1.43808900	-0.96344200	4.18204600
H	3.16558100	-1.18511300	4.58843000
C	3.77546600	1.50644300	4.09932100
H	4.59116300	0.88258500	4.47406400
H	4.16932100	2.12918300	3.29679900
H	3.42029000	2.14469600	4.91523700
C	2.03132400	0.80801500	2.48969200
C	2.39121500	1.99087100	1.59282600
H	3.39108600	1.86226900	1.15953500
H	2.36611400	2.93291300	2.15385500
C	1.45390500	3.19361400	-0.25620700
H	1.37523500	4.08568800	0.37941100
H	2.39318200	3.22693400	-0.81695600
C	0.26142200	3.09047100	-1.20017200
C	1.04082000	5.12679100	-2.34461700
H	1.57226100	5.38819400	-1.42937400
H	1.76052400	4.85343600	-3.12361800

H	0.48223400	6.00696800	-2.67010700
C	-0.98185500	3.91648200	-3.12165300
H	-1.56278200	3.01679400	-2.93349700
H	-1.62564800	4.79919700	-3.06537100
H	-0.53698900	3.86290400	-4.12014200
C	-2.26594900	2.87618700	3.65486700
H	-2.90849700	2.69296900	4.52084500
H	-1.38897200	2.23464800	3.70514000
H	-1.96366700	3.92839200	3.65687300
C	-4.35587100	3.19532300	2.35303800
H	-4.27779800	4.23547700	2.67972500
H	-4.74456800	3.19223100	1.33518300
H	-5.05558600	2.67279100	3.01387700
C	-2.51601000	1.77937300	1.49583600
C	-3.35548700	1.44596400	0.26505500
H	-3.45243700	2.32712500	-0.38402700
H	-4.35870300	1.10373500	0.54706400
C	-3.33965600	-0.10737300	-1.54890100
H	-4.33892000	-0.46304700	-1.26483300
H	-3.45034300	0.67222200	-2.31443800
C	-2.46986700	-1.25765600	-2.05244500
C	-4.06959000	-1.70052600	-3.88747700
H	-4.60873300	-2.64737800	-3.98528900
H	-3.83297400	-1.32549600	-4.88795700
H	-4.71911800	-0.98589300	-3.38380600
C	-1.95665300	-2.98968700	-3.67745000
H	-0.95378200	-2.87774000	-3.27072800
H	-2.36355300	-3.97428600	-3.42400100
H	-1.92197900	-2.89154000	-4.76523600
C	-3.01634600	-2.99731700	3.04734000
H	-2.92054500	-3.38360100	4.06630400
H	-2.88961500	-1.91709000	3.05000900
H	-4.00694400	-3.25947100	2.66251200
C	-1.90251500	-5.07896700	2.27619700
H	-2.91820800	-5.48166900	2.25277900
H	-1.35756900	-5.49637400	1.42983300
H	-1.42420700	-5.39110900	3.21070400
C	-1.15839300	-2.85845800	1.47988200
C	-0.05374400	-3.53183400	0.66703800
H	-0.47717600	-4.08006200	-0.18481600
H	0.52448100	-4.22888200	1.28499700
C	2.01537400	-2.92415000	-0.38478900
H	2.49770900	-3.65690900	0.27358000
H	1.81876800	-3.39393300	-1.35671600
C	2.87977700	-1.67587300	-0.54900900
C	4.69474100	-3.07011200	-1.47855800
H	4.66406100	-3.12980500	-2.57158200
H	5.73665500	-3.10984600	-1.15122300
H	4.17390700	-3.92782900	-1.05416800
C	4.92937100	-0.61062800	-1.31859400
H	5.83755800	-0.64045100	-0.70915500

H	5.20298200	-0.61737700	-2.37719300
H	4.35878500	0.28966800	-1.10489700
N	2.69130800	0.63040800	3.62883300
N	0.08977900	4.02541200	-2.12320200
N	-3.02215000	2.57851500	2.42956900
N	-2.82495600	-1.93090700	-3.13856300
N	-1.97954200	-3.61115200	2.20437500
N	4.10842000	-1.79715100	-1.03287100
O	1.10490200	0.04028700	2.11029500
O	1.40894300	2.02302600	0.56189500
O	-0.53930900	2.12285300	-1.03473100
O	-1.36121800	1.27910100	1.58079900
O	-2.66333700	0.40445700	-0.40793600
O	-1.42172500	-1.51613300	-1.39722900
O	-1.24684900	-1.60064100	1.43254600
O	0.79403100	-2.48312100	0.21004900
O	2.37349400	-0.56819200	-0.21031300
U	-0.05416700	-0.03037700	-0.00638400
N	1.74936800	0.29457800	-2.76329000
O	2.03514400	1.48171100	-2.60151800
O	2.39524100	-0.51422700	-3.40279600

5. NO₃⁻-U(IV)-TMDGA (bidentate)

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TMDGA&NO₃⁻ (bi)

O	0.54111800	-1.83145700	-1.90436200
C	-0.74320900	2.86030700	4.02929200
H	-0.83349400	2.69570700	5.10706600
H	0.10743400	2.30395000	3.64145500
H	-0.60829200	3.93181700	3.84804700
C	-3.22382000	2.87928600	3.96815100
H	-3.11270100	3.94294700	4.19409200
H	-4.06513000	2.76881600	3.28494800
H	-3.43629200	2.34434300	4.89997800
C	-1.91192200	1.56441700	2.33131900
C	-3.21131900	1.04874700	1.71737400
H	-3.71927500	1.86127700	1.17541600
H	-3.89509300	0.66901300	2.48778200
C	-3.83900800	-0.48517600	0.00497100
H	-4.56066000	-1.07893400	0.58138300
H	-4.38539800	0.33009100	-0.49314300
C	-3.11013200	-1.33986500	-1.02926100
C	-5.26056200	-2.17504200	-1.91530500
H	-5.72264800	-1.40240600	-1.30225200
H	-5.59126400	-2.03732300	-2.94855100
H	-5.59413000	-3.15866200	-1.56942900
C	-3.09793800	-2.94476800	-2.86180700
H	-2.03191400	-2.96368200	-2.64676800
H	-3.50692500	-3.95748800	-2.80715200
H	-3.26742700	-2.54810100	-3.86773000
C	-1.82880700	-3.26931800	3.47172200

H	-1.69696800	-3.18006000	4.55442700
H	-2.18842200	-2.32878000	3.06094500
H	-2.54869400	-4.06787300	3.26868100
C	0.06788600	-4.86089500	3.33841900
H	-0.67299000	-5.66237400	3.27200000
H	0.93444500	-5.14749400	2.74489300
H	0.36889500	-4.74553200	4.38457100
C	0.01170800	-2.81697400	1.94583500
C	1.35500500	-3.18662400	1.32909000
H	1.25597200	-4.09761400	0.72146100
H	2.11393100	-3.36454800	2.10179500
C	2.89237400	-2.34781800	-0.26793800
H	3.74662100	-2.54276700	0.39408600
H	2.72662000	-3.22704600	-0.90214600
C	3.14327000	-1.11325100	-1.12890000
C	5.08585600	-2.26296000	-2.15437600
H	6.10745900	-1.87748000	-2.20962300
H	4.86038200	-2.79669800	-3.08359700
H	5.03212800	-2.95861000	-1.31804900
C	4.38541600	-0.00983400	-2.90965000
H	3.52869300	0.66017300	-2.88433800
H	5.29571300	0.53003700	-2.62875200
H	4.50868000	-0.40465200	-3.92201900
C	3.80297800	1.02655100	3.29065100
H	3.84498100	1.63373200	4.20002100
H	3.00198900	0.29525200	3.37357700
H	4.76377200	0.51715900	3.16547600
C	4.47068400	3.04371500	2.00824700
H	5.49022900	2.69375700	2.18952200
H	4.43876400	3.47729700	1.00902800
H	4.23069400	3.81467000	2.74842200
C	2.52876400	1.67123400	1.31638700
C	2.27599100	2.63794400	0.15917300
H	3.06615700	2.55123200	-0.59659800
H	2.22993900	3.67558600	0.51086700
C	0.52104400	3.15487700	-1.39683000
H	0.57905000	4.18911200	-1.03544300
H	1.11433100	3.06198400	-2.31477100
C	-0.93018600	2.73694400	-1.63461200
C	-1.18560200	4.57665300	-3.27347700
H	-1.15803200	4.32429600	-4.33811600
H	-1.87401200	5.41408800	-3.12688700
H	-0.19091300	4.88885300	-2.95977800
C	-3.04579000	3.01502200	-2.80505600
H	-3.73774400	3.79639600	-2.47487000
H	-3.15205300	2.88119600	-3.88548000
H	-3.26708200	2.07986200	-2.29654100
N	-1.97005600	2.39369100	3.37107800
N	-3.79247500	-2.10055500	-1.87430600
N	-0.53935800	-3.61097200	2.85381600
N	4.16115500	-1.13130500	-1.98644200

N	3.55250200	1.90201500	2.13686100
N	-1.66548500	3.41737000	-2.50589200
O	-0.82026600	1.18414700	1.83081800
O	-2.81990100	0.02015500	0.83840300
O	-1.84859600	-1.28639800	-1.04070800
O	-0.54221200	-1.74909600	1.55074500
O	1.73241400	-2.08580600	0.51674500
O	2.37688900	-0.12032700	-1.00289800
O	1.75190200	0.69121300	1.44999100
O	1.01644000	2.27083100	-0.39431600
O	-1.36946300	1.75195400	-0.97647400
U	0.00685300	-0.09835400	-0.09808100
N	0.39076200	-1.01160700	-2.87709700
O	0.51231700	-1.31150500	-4.03534200
O	0.08995600	0.19560700	-2.49649100

6. 3ClO₄-U(IV)-TMDGA

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TMDGA&3ClO₄-

Cl	6.27010047	23.82860186	11.04090086
O	5.81990043	24.76190193	12.05050094
O	5.28200041	22.82660177	10.81470082
O	7.41130057	23.25750181	11.62800090
O	6.47520052	24.57250188	9.91850078
Cl	14.80750112	26.22310203	6.86180054
O	15.86040123	25.31730197	7.18500057
O	14.64890115	26.30350204	5.46510042
O	15.15940119	27.53680212	7.34030054
O	13.59150102	25.81320196	7.49090058
C	7.78470058	20.54020156	8.79340068
H	6.92560053	20.94140163	8.64280065
H	8.45960065	21.05100160	8.33940063
H	7.78070058	19.64130150	8.45740065
C	7.06790052	19.86230153	11.05010088
H	6.96090051	18.95410145	10.76010084
H	7.35510057	19.87530151	11.96500092
H	6.22980050	20.32480155	10.97120086
C	9.10840069	21.14010160	10.69980083
C	9.37600070	21.09930161	12.18190094
H	9.52100072	20.18730156	12.47870096
H	8.62670064	21.47070165	12.67390095
C	10.86820085	22.04090167	13.74960108
H	10.17110079	22.53310171	14.21120107
H	10.97270082	21.17540164	14.17810109
C	12.15020095	22.79690175	13.77890105
C	12.24680093	22.59630172	16.19240127
H	12.72200099	21.81060167	16.46730128
H	12.36820097	23.29090178	16.84410131
H	11.31210087	22.39380172	16.11140122
C	14.01320110	23.75900182	14.90300116
H	13.84610105	24.70250189	14.94080114

H	14.53540109	23.49520183	15.66640120
H	14.49490109	23.55090181	14.09950107
C	12.99100100	18.17030141	10.82410081
H	12.94270098	17.91950140	11.74990090
H	12.15940096	18.56770141	10.55680084
H	13.15940102	17.39020133	10.29150079
C	15.42310117	18.58820142	10.63550082
H	15.54320117	18.03470138	9.86000077
H	16.05890123	19.30690149	10.61610081
H	15.55620120	18.06250139	11.42740087
C	13.80560105	20.40460158	10.56360082
C	14.92310116	21.40570164	10.49580083
H	15.50790119	21.21630164	9.74420075
H	15.44790116	21.38900166	11.31090086
C	15.21290117	23.74220182	10.22350077
H	15.87350123	23.69580181	10.93300083
H	15.67110120	23.71250185	9.36860074
C	14.40220109	24.99970191	10.34170082
C	16.44530127	26.30720205	10.29420081
H	16.64630126	27.05760206	9.72970077
H	16.82130129	26.45400201	11.16520084
H	16.82130129	25.51040198	9.91340079
C	14.21810107	27.37520213	10.55150081
H	13.29510101	27.15230209	10.68630083
H	14.54060111	27.87300213	11.30700087
H	14.30690109	27.90640215	9.75790073
C	13.35650102	22.54430174	5.79790047
H	14.10190110	23.06250179	5.48680045
H	13.60320102	22.07990172	6.60080053
H	13.10320102	21.90910166	5.12430040
C	11.78210092	24.29390186	4.96450038
H	11.89960091	23.83330185	4.13170032
H	10.85390084	24.50560186	5.08460039
H	12.29770096	25.10370191	4.95810038
C	11.76510088	23.53240182	7.27090053
C	10.69330084	24.53530188	7.54480056
H	9.87610077	24.29390186	7.08150054
H	10.97010086	25.41760196	7.24860058
C	9.53920071	25.49370194	9.39490075
H	9.78600073	26.37780202	9.07890070
H	8.65670065	25.27830193	9.05640072
C	9.55490072	25.44910198	10.89020081
C	7.91130063	27.25070212	10.92020083
H	7.81340061	27.03530205	9.98940075
H	7.05100056	27.23220208	11.34580089
H	8.29380063	28.12550217	11.00830085
C	8.81990066	26.29240202	13.00500102
H	9.25200072	27.09660210	13.30280102
H	7.92170060	26.26820200	13.34070101
H	9.30290074	25.52900198	13.33150105
N	8.06530063	20.52350157	10.21610081

N	12.75600100	23.04390179	14.91020115
N	14.07580107	19.13420148	10.63680080
N	14.99490115	26.15680199	10.40790079
N	12.23640096	23.42650181	6.07620045
N	8.79640070	26.26260204	11.55970089
O	9.94130076	21.75880167	9.96770077
O	10.54450080	21.88160170	12.38900097
O	12.64370096	23.19550176	12.67480097
O	12.62670098	20.84280162	10.54740080
O	14.29120109	22.67260172	10.33150082
O	13.13980103	24.88710193	10.37210078
O	12.19330095	22.83570177	8.23660065
O	10.49220078	24.52290188	8.95680067
O	10.33040082	24.61130189	11.44150090
U	11.79370090	23.03220179	10.53200079
Cl	14.57580113	19.73600153	14.30300110
O	15.69850120	20.23560158	13.70720107
O	14.48970113	18.33180139	14.10140108
O	14.54060111	20.05920156	15.69220119
O	13.44130104	20.25230157	13.67320107