Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary information

The Coordination of Amidoxime Ligands with Uranyl in the Gas Phase: A Mass Spectrometry and DFT Study

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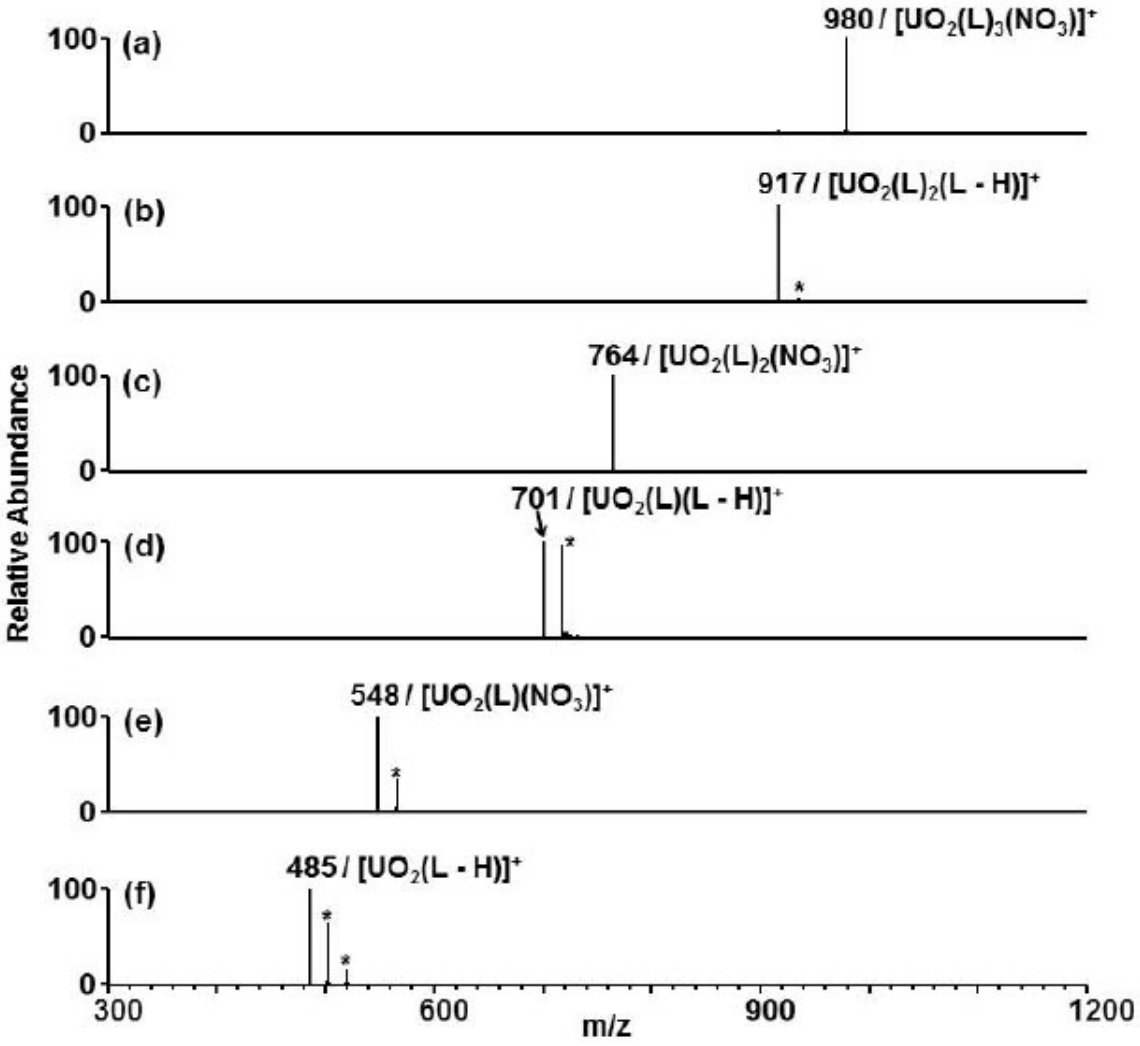

Figure S1. The hydration results of the uranyl-NAO complexes: (a) $[UO_2(L)_3(NO_3)]^+$, (b) $[UO_2(L)_2(L - H)]^+$, (c) $[UO_2(L)_2(NO_3)]^+$, (d) $[UO_2(L)(L - H)]^+$, (e) $[UO_2(L)(NO_3)]^+$, and (f) $[UO_2(NO_3)]^+$. The isolation width was 2 *Dalton,* and the reaction time was 30 *s* for all the ions.

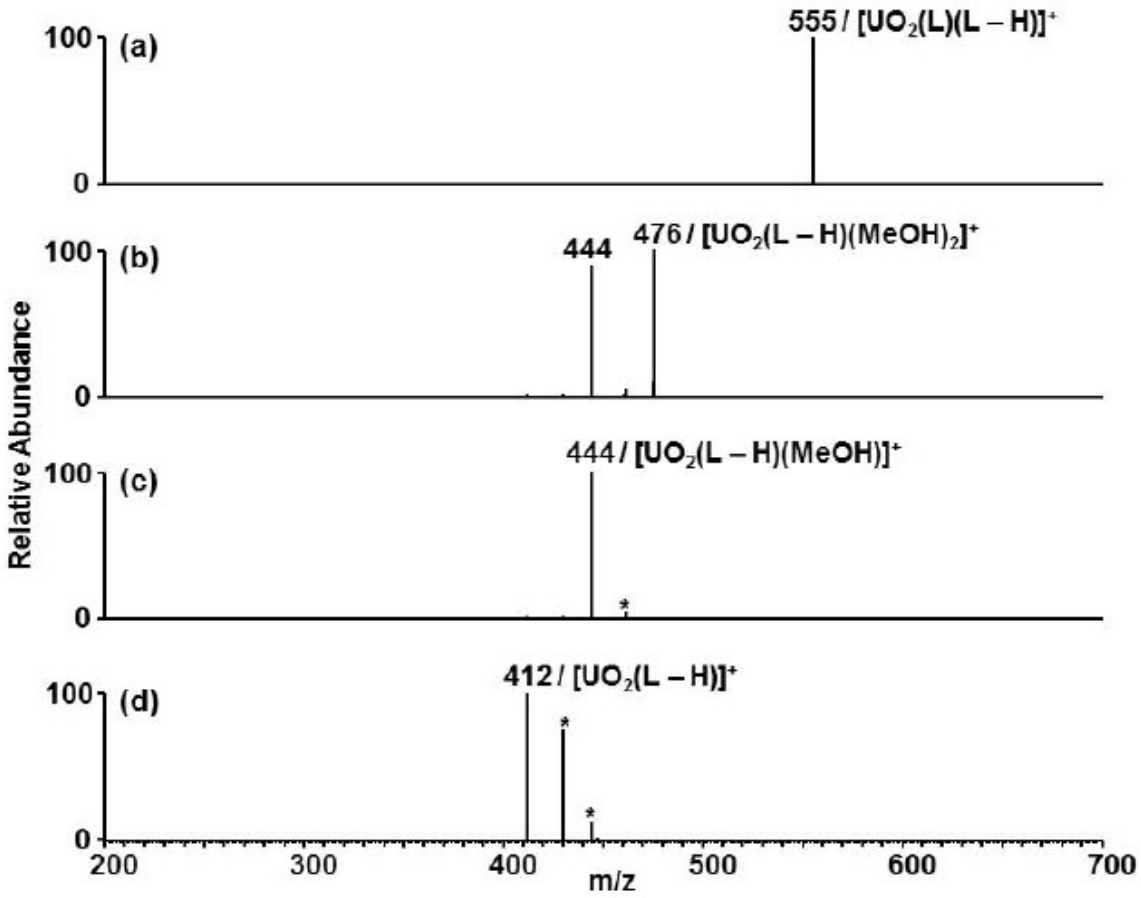

Figure S2. The hydration results of the uranyl-GIO complexes: (a) $[UO_2(L)(L - H)]^+$, (b) $[UO_2(L - H)(MeOH)_2]^+$, (c) $[UO_2(L - H)(MeOH)]^+$, and (d) $[UO_2(L - H)]^+$. The isolation width was 2 *Dalton,* and the reaction time was 30 *s* for all the ions.

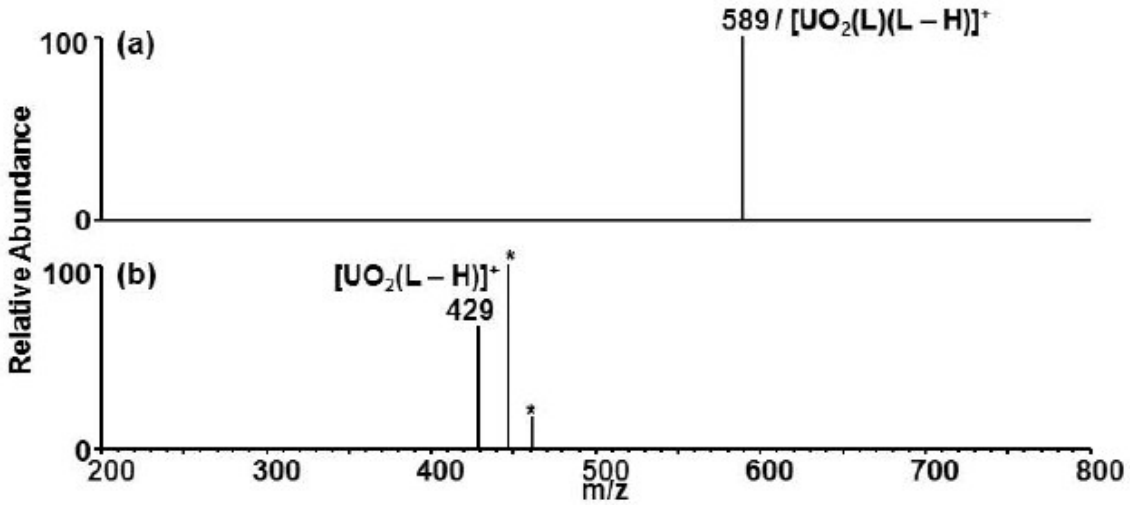

Figure S3. The hydration results of the uranyl-GDO complexes: (a) $[UO_2(L)(L - H)]^+$, and (b) $[UO_2(L - H)]^+$. The isolation width was 2 *Dalton,* and the reaction time was 30 *s* for all the ions.

Cartesian Coordinates of all species

Figure 4 (a): $[UO_2(NAO - H)]^+$

U	-2.77696500	-0.60166500	0.19449500
O	-2.96197700	0.22060000	1.73561700
O	-2.71569300	-1.73889600	-1.14126800
O	-2.59579000	1.19151600	-0.97560600
N	-1.28087300	0.86099300	-0.64358800
C	-0.41102000	1.86537100	-0.59094300
N	-0.81125400	3.11412800	-0.83192600
H	-1.78451700	3.28853900	-1.03908300
H	-0.13882800	3.85093200	-0.97130100
C	4.80765200	-1.43020900	-0.55709000
C	3.49188700	-1.15595600	-0.83062900
C	2.88621300	0.05225100	-0.39901900
C	3.68739300	0.99904000	0.32561200
C	5.02972700	0.70023200	0.59927500
C	5.59423300	-0.49418300	0.16921500
H	0.95157800	-0.34392800	-1.25859800
H	5.24238500	-2.35878100	-0.89998200
H	2.90014600	-1.87225300	-1.39012400
C	1.53940100	0.35474400	-0.67404200
C	3.08242000	2.22312600	0.73728800
H	5.65239000	1.39884400	1.14455500
C	1.77677300	2.50329400	0.44520300
C	0.97883800	1.55879900	-0.26699200
H	3.67593000	2.93566900	1.29835800
H	1.33525200	3.42840300	0.79731900
O	6.88825800	-0.68446300	0.47840100
C	7.55807200	-1.87745100	0.05700500
H	7.56922400	-1.95913200	-1.03344600
H	8.57709800	-1.77951300	0.42295600
H	7.09710300	-2.76583100	0.49791200

Figure 4 (b): $[UO_2(NAO)(NO_3)]^+$

U	2.72332300	0.12910100	-0.06798800
O	2.20706300	-1.94055700	-0.85431100
N	0.90461300	-1.47723500	-0.81753900
C	0.01778000	-2.19962200	-0.01148100
N	0.56004200	-3.17953100	0.67637600
H	1.53913400	-3.39138900	0.51190700
H	0.04701300	-3.66396900	1.39687900
C	-4.91478700	1.44709800	-0.42073600
C	-3.58908900	1.11260100	-0.49662900
C	-3.14779800	-0.20929300	-0.21596000
C	-4.12239900	-1.19489000	0.17146000
C	-5.47034700	-0.83635500	0.24228200
C	-5.87635200	0.46455700	-0.04940100
H	-1.07701100	0.20982000	-0.53396800
H	-5.22524500	2.45908500	-0.63979800
H	-2.85720800	1.86403200	-0.77061200
C	-1.79560100	-0.56352700	-0.29164200
C	-3.66658900	-2.51554400	0.47462100
H	-6.22441000	-1.55860900	0.52948000
C	-2.34485000	-2.83986800	0.41390600
C	-1.37369100	-1.85976000	0.02186600
H	-4.39636600	-3.26907900	0.74643000
H	-2.03905500	-3.86075500	0.61123000
O	-7.18782500	0.70628100	0.04904600
C	-7.70823600	2.01507200	-0.22724000
H	-7.50546100	2.30612900	-1.26100800
H	-8.78133000	1.93278900	-0.07605900
H	-7.29669400	2.75384600	0.46511700
H	0.53562600	-1.27151600	-1.74564200
N	1.32293600	2.55129800	0.59023400
O	2.59458200	2.42162400	0.73228900
O	0.75224200	1.46561900	0.14258000
O	0.71930200	3.54292000	0.83503000
O	2.59414500	-0.47654700	1.57778300
O	2.96722600	0.70913400	-1.70602400

Figure 4 (c): $[UO_2(NAO)(NAO - H)]^+$

U	-6.27615000	-3.28568800	-4.57850800
O	-7.52426700	-4.53088400	-4.72071300
O	-4.94107800	-2.19273000	-4.12722000
O	-4.63168200	-4.76274700	-5.06514600
N	-3.30678500	-4.46338400	-5.08490900
C	-2.42845200	-5.37090500	-5.46538300
N	-2.87147100	-6.59764600	-5.74450700
H	-3.86284000	-6.78076600	-5.67139500
H	-2.27288300	-7.25672500	-6.21332100
C	2.51619100	-1.87104300	-6.68542200

C	1.18209300	-2.17967900	-6.59622000
C	0.75018800	-3.44037900	-6.11402900
C	1.74323800	-4.40167000	-5.72686300
C	3.10382600	-4.06745100	-5.82571300
C	3.49670500	-2.82358900	-6.29536900
H	-1.35276000	-3.05762400	-6.35174200
H	2.81512900	-0.89979500	-7.05463300
H	0.44111500	-1.44701400	-6.89680800
C	-0.61534500	-3.77905200	-6.01507900
C	1.30691400	-5.67306800	-5.25464600
H	3.86912200	-4.77789100	-5.53803900
C	-0.02274000	-5.98183800	-5.17144300
C	-1.00849000	-5.02396900	-5.55148300
H	2.05050900	-6.40001500	-4.94886900
H	-0.32968300	-6.94434400	-4.77906300
O	4.82448200	-2.59883800	-6.35244200
C	5.31338500	-1.34128900	-6.82440100
H	4.97404000	-0.51931100	-6.18717300
H	6.39705300	-1.41466200	-6.77146100
H	5.01241200	-1.16195100	-7.86078600
H	-3.03026800	-3.55461800	-4.72562200
N	-7.56170400	-1.59880300	-5.59633200
C	-8.18712800	-0.52852000	-6.01340400
N	-8.83063900	0.21555200	-5.06632900
H	-8.85344100	-0.13375400	-4.12076600
H	-9.63466700	0.74957500	-5.35670600
C	-8.48456300	-0.83446400	-12.19470300
C	-8.36610500	-1.31143500	-10.91273100
C	-8.34920800	-0.43569200	-9.79831800
C	-8.46321800	0.97336700	-10.03725100
C	-8.58006200	1.44400400	-11.35697200
C	-8.59322700	0.56301000	-12.42579000
H	-8.13985500	-1.97739500	-8.30956000
H	-8.49592800	-1.52889100	-13.02339800
H	-8.28499200	-2.37946700	-10.74241400
C	-8.22801400	-0.91255000	-8.47580500
C	-8.44973300	1.84883400	-8.91454500
H	-8.66590000	2.50492100	-11.55869000
C	-8.34808000	1.36253700	-7.64024000
C	-8.23604100	-0.04078400	-7.40012500
H	-8.51456900	2.91782900	-9.08336700
H	-8.31376400	2.05088800	-6.80446100
O	-8.71308300	1.11472600	-13.65483400
C	-8.74949000	0.27277400	-14.80608700
H	-9.60521300	-0.40879000	-14.77550400
H	-8.85619500	0.94531700	-15.65438500
H	-7.82205100	-0.29863200	-14.91256000
O	-6.73019800	-2.29600900	-6.45700400

Figure 4 (d): $[UO_2(NAO)_2(NO_3)]^+$

U	-5.01387200	-2.18953900	-1.93468400
O	-6.63336100	-3.62113200	-2.66718500
N	-6.45147700	-4.95971700	-2.80513000
C	-7.48463000	-5.75431600	-3.00539200
N	-8.70422100	-5.21395300	-3.00918500
H	-8.79116200	-4.21834100	-2.85907900
H	-9.49356100	-5.74553600	-3.33544700
C	-4.70002400	-10.89299900	-5.01606400
C	-4.88578900	-9.54360900	-4.84895900
C	-5.98117300	-9.03907400	-4.10489800
C	-6.90764100	-9.97379800	-3.53228900
C	-6.70122900	-11.35118800	-3.71517800
C	-5.61700400	-11.81589100	-4.44332800
H	-5.50388700	-6.96075700	-4.38981600
H	-3.85191300	-11.24754900	-5.58535400
H	-4.18087500	-8.84690000	-5.28932400
C	-6.19015400	-7.65654700	-3.91849000
C	-8.01435900	-9.46425800	-2.79402900
H	-7.38779700	-12.07334900	-3.29055700
C	-8.20008800	-8.11921200	-2.63020100
C	-7.27498700	-7.19171100	-3.19364600
H	-8.71149700	-10.16437700	-2.34826500
H	-9.03129500	-7.75737800	-2.03624200
O	-5.50676700	-13.15431200	-4.56206000
C	-4.41690400	-13.71566000	-5.29671300
H	-3.45603100	-13.45335400	-4.84410600
H	-4.55766900	-14.79269900	-5.24417300
H	-4.43800100	-13.39806500	-6.34342600
H	-5.52100800	-5.32045400	-2.61407700
O	-3.73364200	-1.16409000	-3.48637000
N	-3.76941500	0.05111400	-4.08064900
C	-3.14718200	1.10845900	-3.58938600

N	-2.46237100	1.01678700	-2.45218700
H	-2.44655700	0.15832700	-1.91454300
H	-2.18169100	1.86415800	-1.98541300
C	-5.75317600	5.68625500	-6.83093100
C	-5.69682500	4.48749700	-6.16440100
C	-4.48854500	4.02168900	-5.58985300
C	-3.31532000	4.83889400	-5.70943700
C	-3.39249700	6.06243200	-6.39645600
C	-4.58746800	6.48995000	-6.95292500
H	-5.31237200	2.20718200	-4.77073600
H	-6.69018300	6.01382700	-7.25963100
H	-6.59228800	3.88235700	-6.07354800
C	-4.40880500	2.79488500	-4.89541600
C	-2.10543100	4.37869000	-5.11498300
H	-2.51845100	6.69404800	-6.49834800
C	-2.05277200	3.18995800	-4.44010500
C	-3.21762700	2.37581200	-4.32865200
H	-1.21265900	4.98603000	-5.21010000
H	-1.11564500	2.84761400	-4.01701600
O	-4.55875500	7.67899700	-7.58985100
C	-5.75094000	8.19472300	-8.18442000
H	-6.53125700	8.35697500	-7.43482500
H	-5.46674200	9.14964000	-8.62043300
H	-6.12059500	7.53251300	-8.97314200
H	-4.10024800	0.06591600	-5.03694600
N	-3.93100800	-1.36144700	0.64487700
O	-4.96044400	-2.12150100	0.51260700
O	-3.41158200	-0.99998800	-0.48712200
O	-3.49289300	-1.01829400	1.69877500
O	-3.99495700	-3.64383200	-1.95567100
O	-6.12792800	-0.81946800	-1.98501500

Figure 4 (e): $[UO_2(NAO)_2(NAO - H)]^+$

U	-0.70133400	-0.15747600	-1.05282700
N	-3.63149400	-1.44388400	-0.59965400
C	-4.62546600	-2.29107400	-0.73747000
N	-4.37295600	-3.46257300	-1.33652100
H	-3.44074100	-3.60457900	-1.70158000
H	-5.13378100	-4.02681700	-1.67490100
C	-9.52137000	1.24989200	0.58249600
C	-8.26923900	0.95884600	0.10062200
C	-7.73498100	-0.35062300	0.18440500
C	-8.53805900	-1.37919700	0.77973700
C	-9.81794400	-1.06176600	1.26703300
C	-10.31176700	0.22926100	1.17601600
H	-5.87137700	0.10646400	-0.79141200
H	-9.89994200	2.25980700	0.50582500
H	-7.67276600	1.74392000	-0.35117900
C	-6.45102100	-0.67245800	-0.30706400
C	-8.00379100	-2.69730700	0.85316400
H	-10.43990100	-1.82385400	1.72063800
C	-6.75720400	-2.98562300	0.36902800
C	-5.95785800	-1.96240500	-0.21907600
H	-8.60027200	-3.47794600	1.31139500
H	-6.35916100	-3.98924100	0.46284500
O	-11.55138500	0.43246600	1.67302800
C	-12.13291400	1.73504000	1.61227700
H	-12.24639400	2.07289200	0.57767700
H	-13.11559300	1.63506900	2.06767200
H	-11.54342700	2.46144300	2.18003300
O	0.61551500	-0.61826100	0.81106000
N	1.68180400	-1.44398100	0.71745200
C	2.45875700	-1.65334900	1.75532000
N	2.11423100	-1.08714800	2.91988800
H	1.30356300	-0.48250300	2.91771600
H	2.78782900	-1.01633200	3.66331000
C	7.42025300	-4.18211600	-0.93817500
C	6.31981200	-3.36789700	-0.83407000
C	5.53220600	-3.34280700	0.34333100
C	5.91467500	-4.18561500	1.43900300
C	7.04581900	-5.01118100	1.31419700
C	7.79344900	-5.01872300	0.14805500
H	4.14126900	-1.85580900	-0.35241800
H	7.99840000	-4.18194100	-1.85193700
H	6.04090800	-2.73434400	-1.66906500
C	4.39588200	-2.51464500	0.47128300
C	5.12464000	-4.15458600	2.62337400
H	7.35033600	-5.65625800	2.12938500
C	4.02593300	-3.34532600	2.72275300
C	3.64372600	-2.50994400	1.63290000
H	5.39993700	-4.79711000	3.45194600
H	3.42055200	-3.36506800	3.62139200

O	8.86012500	-5.84716900	0.12584100
C	9.67780600	-5.91623500	-1.04270200
H	10.14239100	-4.94996100	-1.26166500
H	10.45274300	-6.64350600	-0.81135400
H	9.10564200	-6.26062100	-1.90954800
H	1.80429700	-1.92712400	-0.16974600
O	-0.85274100	1.21379100	-2.80854600
N	0.18126900	1.79162500	-2.08688800
C	0.47999500	3.02051300	-2.39614800
N	-0.23227000	3.69659500	-3.33306200
H	-0.91737000	3.15324600	-3.83909600
H	0.19801000	4.47459400	-3.80508800
C	6.03200400	3.62860200	0.28731700
C	4.99827800	2.98066900	-0.34548000
C	3.80319200	3.65655400	-0.69220400
C	3.69517000	5.04952600	-0.37300000
C	4.76368400	5.69605100	0.27842000
C	5.91691200	5.00685700	0.60699400
H	2.82444200	1.96294000	-1.61539100
H	6.93216900	3.08264300	0.53454700
H	5.09681600	1.92862200	-0.59186300
C	2.73162000	3.01028200	-1.35198600
C	2.50191300	5.73388100	-0.73761000
H	4.69967800	6.74866200	0.52705000
C	1.48286400	5.08523600	-1.38227200
C	1.58629600	3.69942500	-1.69619400
H	2.40622600	6.78549800	-0.49113000
H	0.57353100	5.61918800	-1.63216700
O	6.88853000	5.72013000	1.23067900
C	8.11837600	5.08455200	1.56485200
H	8.63290900	4.71241500	0.67287000
H	8.72710200	5.85468100	2.03420100
H	7.96726800	4.26374300	2.27396300
H	-3.70940800	-0.58920400	-0.05310400
O	-2.41669900	-1.71855500	-1.12938000
O	-1.87893800	0.77562100	-0.07549100
O	0.45072400	-1.28146600	-1.84443200

Figure 4 (f): $[UO_2(NAO)_3(NO_3)]^+$

U	0.64115400	0.42601800	0.93220700
N	-2.68887400	0.70990000	1.02262100
C	-3.44446700	0.05931500	1.88391200
N	-2.96896400	-0.26171600	3.08578000
H	-1.98729300	-0.13655400	3.32088000
H	-3.59366300	-0.64270000	3.77577300
C	-9.08335400	0.78734900	-0.56650200
C	-7.80289200	1.14314000	-0.22016900
C	-6.94332700	0.23879300	0.44988600
C	-7.44308800	-1.06590700	0.77183300
C	-8.75706100	-1.41219300	0.40845000
C	-9.57278500	-0.50808800	-0.25077100
H	-5.27199800	1.59018600	0.61209800
H	-9.71460700	1.50079500	-1.07799500
H	-7.43881200	2.13578900	-0.46232500
C	-5.62421200	0.58528900	0.82119000
C	-6.58339500	-1.96912600	1.45957200
H	-9.15337800	-2.39269000	0.64307300
C	-5.31119500	-1.60867200	1.81169500
C	-4.81253100	-0.31399800	1.48749800
H	-6.95073500	-2.96090800	1.69767100
H	-4.66463500	-2.32040700	2.31167100
O	10.81884600	-0.93586400	-0.55518200
C	11.72245300	-0.05772000	-1.22519500
H	11.34198500	0.23088200	-2.20998400
H	12.64183700	-0.62593100	-1.34788900
H	11.92709500	0.83619500	-0.62790800
O	0.61085200	1.71908600	-1.01432200
N	1.04572000	2.99593800	-0.95644000
C	1.01969500	3.76677900	-2.01719700
N	0.46292800	3.27559700	-3.13686000
H	0.15874300	2.31202700	-3.10980400
H	0.65236700	3.71378400	-4.02207000
C	4.84688100	8.32254800	-0.33069800
C	4.35613800	7.04134800	-0.38032500
C	3.20357900	6.72418900	-1.14063100
C	2.55727500	7.77505700	-1.87205200
C	3.07573600	9.08045600	-1.81011100
C	4.20132300	9.36157500	-1.05329900
H	3.20506900	4.62236500	-0.67787500
H	5.72597800	8.53331600	0.26246300
H	4.85418800	6.25442400	0.17549200
C	2.68248400	5.41356600	-1.20538600

C	1.40311800	7.45207500	-2.64122700
H	2.60179700	9.88847500	-2.35411300
C	0.91555500	6.17455500	-2.68732500
C	1.55591000	5.13076800	-1.95774200
H	0.90190100	8.24275100	-3.18793000
H	0.01677700	5.95929900	-3.25332100
O	4.61977800	10.64627300	-1.05718000
C	5.77098500	11.01742100	-0.29863600
H	6.66467200	10.48999900	-0.64602900
H	5.89607300	12.08490700	-0.46566900
H	5.62074300	10.83375700	0.76963200
H	1.32769000	3.33668300	-0.03912700
O	2.74494500	-0.24245600	0.10845600
N	3.33161500	-1.42011600	0.38735400
C	3.90590200	-2.13272200	-0.55112900
N	3.95912100	-1.61192800	-1.78972800
H	3.47462900	-0.73556200	-1.92928400
H	4.12217300	-2.21867300	-2.57506400
C	4.50392500	-7.60593700	2.26680800
C	3.93099100	-6.39197600	1.97810000
C	4.49898300	-5.52084600	1.01605000
C	5.69092400	-5.93798300	0.33659100
C	6.26116000	-7.18623700	0.64387300
C	5.68610300	-8.01418900	1.59321400
H	3.00483300	-3.98232100	1.20168400
H	4.04931000	-8.24586500	3.01045500
H	3.02978400	-6.08628400	2.49829200
C	3.92620600	-4.26813300	0.70508200
C	6.25852200	-5.06182600	-0.63164900
H	7.16196700	-7.51906400	0.14260400
C	5.68798900	-3.85032900	-0.91240900
C	4.50397900	-3.43494000	-0.23652600
H	7.16655100	-5.36409100	-1.14102000
H	6.15689500	-3.18487400	-1.62775800
O	6.31147200	-9.19194500	1.81862500
C	5.78718900	-10.09367500	2.79229100
H	4.77950100	-10.42744000	2.52581800
H	6.46086400	-10.94775100	2.78944300
H	5.77903700	-9.64295800	3.78951500
H	-3.01360300	0.84125100	0.07250800
O	-1.48866700	1.22768700	1.33783600
O	1.34348900	1.91075900	1.63372500
O	-0.10576700	-1.00157300	0.18027700
O	0.97349800	-1.80504300	4.49903500
N	0.91197700	-1.13525000	3.50501400
O	-0.07394100	-0.35375100	3.24406400
O	1.81840300	-1.13130600	2.60012400
H	3.33827300	-1.70669700	1.36307600

Figure 5 (a): $[UO_2(GIO - H)]^+$

C	-3.39118100	1.26774300	0.17368000
H	-3.74045800	2.16739100	-0.33718900
H	-3.68591300	1.35887600	1.22612600
N	-1.23765200	-0.00001900	0.11680200
C	-1.89422600	-1.17533900	0.11436700
C	-1.89450500	1.17525500	0.11477100
N	-1.10207900	-2.21656100	0.06273000
N	-1.10272200	2.21663400	0.06159100
O	0.23306900	-2.04198700	0.05744200
O	0.23232600	2.04281000	0.05403000
H	-1.42379700	3.17880300	0.05401400
H	-1.42257500	-3.17890000	0.05475200
U	1.23153300	-0.00001400	-0.03057600
O	1.48508900	0.00140000	1.70506700
O	1.16866700	-0.00114200	-1.78466100
C	-4.01372600	0.00025600	-0.44168200
H	-3.85986200	0.00179200	-1.52390300
H	-5.09002500	-0.00004600	-0.26896000
C	-3.39103900	-1.26869000	0.17021900
H	-3.68769400	-1.36424200	1.22174000
H	-3.73864600	-2.16678000	-0.34457400

Figure 5 (b): $[UO_2(GIO - H)(MeOH)]^+$

C	3.78824000	1.26856500	0.23389100
C	4.42095300	0.00016000	-0.36908400
C	3.78833500	-1.26826200	0.23458800
N	1.63748600	0.00006800	0.14335800
C	2.29174500	1.17405900	0.15067300
C	2.29182400	-1.17385800	0.15078500
N	1.50327900	2.21840800	0.08065900
N	1.50348400	-2.21827400	0.08061700
O	0.16789200	2.06341800	0.04934700

O	0.16810000	-2.06338800	0.04845100
U	-0.85562500	-0.00015700	-0.06539200
O	-1.15616500	-0.00034300	1.67234700
O	-0.74505800	0.00044100	-1.82681300
O	-3.30819000	0.00041700	-0.38661200
H	-3.64750300	0.00095400	-1.29055700
C	-4.41870200	0.00027700	0.56198500
H	-5.01953900	-0.89772000	0.41844000
H	-3.97506600	0.00045500	1.55404800
H	-5.01988100	0.89802100	0.41829800
H	1.83764300	3.17572800	0.07733700
H	1.83777600	-3.17560900	0.07631500
H	4.06873900	1.36139800	1.28998400
H	4.14630900	2.16651200	-0.27413000
H	5.49490200	0.00022500	-0.18123000
H	4.28207900	-0.00024100	-1.45347400
H	4.06859000	-1.36035100	1.29079100
H	4.14667500	-2.16636000	-0.27294400

Figure 5 (c): $[UO_2(GIO - H)(MeOH)_2]^+$

C	3.96564300	-1.29399400	0.04339400
C	4.58647400	0.04301300	0.48536300
C	3.97657500	1.20757000	-0.31463700
N	1.80998600	-0.02823800	-0.09734000
C	2.46654400	-1.18921200	0.07256900
C	2.47636500	1.12776700	-0.26091900
N	1.68635400	-2.22362800	0.26325800
N	1.70599000	2.18088300	-0.37319700
O	0.35110900	-2.09754500	0.25105600
O	0.36911000	2.06904300	-0.36045100
U	-0.71532300	-0.00491400	-0.00629000
O	-0.89446200	-0.25816100	-1.74967400
O	-0.71812400	0.25213100	1.74588300
O	-2.58380400	-1.61504100	0.35351700
H	-2.75527800	-1.86191200	1.27001700
C	-3.05520700	-2.66494700	-0.53436200
H	-4.11937500	-2.83406500	-0.36679100
H	-2.89078100	-2.30786200	-1.54769800
H	-2.48362000	-3.57821600	-0.36598700
H	2.04365100	-3.16111600	0.41050200
H	2.07323000	3.11748200	-0.50014500
H	4.27748800	-1.52770400	-0.98167800
H	4.30546800	-2.11530000	0.67814400
H	5.66633500	0.01692400	0.33617200
H	4.40987500	0.19653800	1.55339300
H	4.29019700	1.14263400	-1.36350600
H	4.32332000	2.17094100	0.06568200
C	-2.80338500	2.80663400	0.67962000
H	-2.62631200	2.44290100	1.68850300
H	-2.12498100	3.63111300	0.45829700
H	-3.84364700	3.11552000	0.57281000
O	-2.53386100	1.69169900	-0.21344900
H	-2.74998200	1.94308900	-1.11932600

Figure 5 (d): $[UO_2(GIO)(GIO - H)]^+$

C	-5.32416900	0.01649800	-1.26956300
C	-5.88695900	0.68414300	-0.00030000
C	-5.32250800	0.01402700	1.26689600
N	-3.17796800	-0.14239700	-0.00293000
C	-3.82658000	-0.06040400	-1.17530300
C	-3.82509100	-0.06339300	1.17033100
N	-3.03730200	-0.04509900	-2.22254200
N	-3.03460700	-0.05150400	2.21678200
O	-1.70453000	-0.17515200	2.08026100
U	-0.66250100	-0.01110500	-0.00335100
C	6.59734900	-0.44185000	0.21399500
C	6.02658200	-1.69916400	-0.45622600
C	4.64515500	-2.02489600	0.13471500
N	4.26730600	0.41560700	0.10542700
C	5.64203900	0.70966300	0.08812900
C	3.75101000	-0.81969300	0.08736700
N	6.06620200	1.90860900	-0.02185500
N	2.44923400	-0.95099400	0.03196900
O	5.00444100	2.81935200	-0.09460700
O	1.64401000	0.13313400	0.02234100
H	5.44668600	3.67105100	-0.17324600
O	-1.70705600	-0.16766300	-2.08811200
O	-0.32604600	-1.76054400	-0.00711900
O	-0.85162900	1.74601300	-0.00072600
H	-3.38307100	0.00835200	-3.17420500
H	-3.37907600	-0.00062100	3.16902600
H	-5.62353100	0.55732000	2.16529100

H	-5.71740400	-1.00500700	1.35778900
H	-6.97537000	0.61679500	0.00037600
H	-5.62748100	1.74625000	0.00056700
H	-5.62680400	0.56126400	-2.16651300
H	-5.71880500	-1.00253200	-1.36160100
H	3.61940500	1.19803000	0.05183000
H	1.98956500	-1.85983000	0.01693900
H	4.16622200	-2.85532700	-0.38882400
H	4.75246300	-2.32383100	1.18417500
H	5.94295600	-1.54690700	-1.53612900
H	6.69512900	-2.54665800	-0.30054800
H	6.77270900	-0.64190300	1.27801700
H	7.55191700	-0.14510300	-0.21914800

Figure 6 (a): $[UO_2(GDO - H)]^+$

O	-1.42068600	1.66643500	0.46492300
N	-0.12349600	1.55760200	0.00246600
C	0.61364200	2.62541600	-0.02970400
N	0.13643800	3.81426400	0.37004500
H	0.67975000	4.65627600	0.28405000
H	-0.83184400	3.87568700	0.65017200
C	2.04105900	2.52690400	-0.51560500
C	2.54189200	1.10733800	-0.81805600
H	2.68452400	3.01260000	0.22743200
H	2.12379600	3.12788800	-1.42753500
C	2.68760200	0.23680700	0.45443900
H	1.86501800	0.62547200	-1.52329200
H	3.51425700	1.18653400	-1.30994500
H	3.53227100	0.58442100	1.05397700
H	1.79578500	0.32630800	1.07648900
N	4.06578600	-1.79413600	0.42382100
H	4.78431000	-1.26711400	0.89212000
H	4.24809000	-2.77402000	0.26285600
C	2.88203500	-1.22127700	0.16321700
N	1.90495400	-1.94107200	-0.34015300
O	0.72266400	-1.45499900	-0.76221000
H	2.04542100	-2.92042200	-0.57193200
U	-1.16885900	-0.49184400	0.03590100
O	-0.63918800	-0.86256200	1.68385400
O	-1.83647300	-0.38534300	-1.59109800

Figure 6 (b): $[UO_2(GDO)(GDO - H)]^+$

O	-1.08009300	2.06937100	0.89253100
N	-2.16711500	1.23927300	0.79280700
C	-3.32325900	1.72825400	1.08899300
N	-3.46995900	3.03885000	1.44004100
H	-4.28899300	3.31311400	1.95781400
H	-2.60604500	3.51693200	1.65882600
C	-4.55943900	0.86830800	0.97925700
C	-4.32691800	-0.53115900	0.39502700
H	-5.30092000	1.41612600	0.38403500
H	-4.99619300	0.76171000	1.97940200
C	-3.89155600	-0.48459800	-1.08780000
H	-3.56261000	-1.04432200	0.97731100
H	-5.25276300	-1.10624900	0.48189500
H	-4.73351400	-0.19086700	-1.72040800
H	-3.10832800	0.26670100	-1.20967200
N	-3.98686200	-2.43745200	-2.58344000
H	-4.72547800	-1.96681400	-3.07800400
H	-3.59249000	-3.25072900	-3.03097300
C	-3.33249100	-1.77390600	-1.60166200
N	-2.22342900	-2.26302800	-1.10844900
O	-1.54909900	-1.77403600	-0.06152200
H	-1.85088000	-3.13339800	-1.48140900
U	-0.11308300	0.11890500	0.22053800
O	1.83108900	1.51398400	0.05447800
N	2.24534200	1.83271700	-1.18002600
C	3.48468600	1.72769700	-1.56670800
N	3.83676500	1.99340200	-2.84710300
C	4.53198700	1.24749200	-0.60242000
H	4.81016700	2.11163700	-3.07128300
H	3.17404200	2.37560600	-3.50457700
C	4.42878700	-0.27926500	-0.30814300
H	4.42473600	1.82164900	0.32080200
H	5.51234000	1.48292600	-1.02103600
C	3.84469300	-0.57184100	1.09398000
H	3.80011200	-0.75252700	-1.06230100
H	5.42321400	-0.72372300	-0.38751500
H	4.61195500	-0.43717300	1.86034200
H	3.04240700	0.14025500	1.29208300
C	3.26053400	-1.94476200	1.22737100
N	3.84069200	-2.84387400	2.05657900

N	2.20636700	-2.27053100	0.52757900
H	3.38193800	-3.71301500	2.28624700
H	4.51020200	-2.51000200	2.72977300
O	1.61033100	-1.47068900	-0.36871300
H	1.78323200	-3.18930800	0.63846500
H	1.50015700	2.07236900	-1.83534900
O	-0.33207500	0.51582900	-1.52384900
O	0.24142100	-0.37233200	1.90117200