Supporting Information

Uncovering the Reduction Mechanism of Np (VI) with N, N-diethyl hydroxylamine: a Scalar-relativistic DFT Investigation

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Table S1. The values of ρ(r) (au), $\nabla^2\rho(r)$ (au), H(r) (au) and MBO of the N/O-H and H-O_{yl} bonds for the structures at the 3rd and 4th stage for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction with $(C_2H_5)_2NOH$ at the B3LYP/ECP60MWB/6-31G(d) level of theory.

	Bond	ρ(r)	$\nabla^2\rho(r)$	H(r)	MBO
$IC3^I$	$O\text{-}H_O$	0.335	-1.812	-0.510	0.664
	$H_O\text{-}O_{yl}$	0.020	0.069	0.000	-
$TS3^I$	$O\text{-}H_O$	0.284	-1.385	-0.402	0.524
	$H\text{-}O_{yl}$	0.051	0.154	-0.003	0.165
$INT3^I$	$O\text{-}H_O$	0.031	0.100	-0.001	0.105
	$H_O\text{-}O_{yl}$	0.309	-1.563	-0.449	0.628
$IC4^I$	$N\text{-}H_N$	0.224	-0.894	-0.274	0.437
	$H_N\text{-}O_{yl}$	0.095	0.174	-0.027	0.249
$TS4^I$	$N\text{-}H_N$	0.219	-0.849	-0.264	0.430
	$H_N\text{-}O_{yl}$	0.099	0.163	-0.032	0.253
$INT4^I$	$N\text{-}H_N$	0.037	0.100	-0.001	0.216
	$H_N\text{-}O_{yl}$	0.298	-1.453	-0.424	0.505
$IC3^{II}$	$N\text{-}H_N$	0.283	-1.377	-0.382	0.546
	$H_N\text{-}O_{yl}$	0.052	0.159	-0.002	0.187
$TS3^{II}$	$N\text{-}H_N$	0.151	-0.232	-0.122	0.348
	$H_N\text{-}O_{yl}$	0.162	-0.254	-0.147	0.314
$INT3^{II}$	$N\text{-}H_N$	0.048	0.126	-0.003	0.229
	$H_N\text{-}O_{yl}$	0.287	-1.357	-0.401	0.483
$IC4^{II}$	$O\text{-}H_O$	0.335	-0.183	-0.513	0.574
	$H_O\text{-}O_{yl}$	0.026	0.088	-0.119	0.105
$TS4^{II}$	$O\text{-}H_O$	0.293	-0.149	-0.427	0.441
	$H_O\text{-}O_{yl}$	0.053	0.164	-0.264	0.226
$INT4^{II}$	$O\text{-}H_O$	0.037	0.029	-0.001	0.159
	$H_O\text{-}O_{yl}$	0.305	-1.536	-0.443	0.563

Table S2. The energy barriers (kcal mol^{-1}) for the hydrolysis reaction of $C_2H_5N(O)C_2H_4$ with n=1-4 water molecules at the B3LYP/6-31G(d) level of theory in the aqueous phase.

	1	2	3	4
TS_h-nw-1	33.7	24.2	24.3	25.1
TS_h-nw-2	31.8	14.3	12.6	14.6

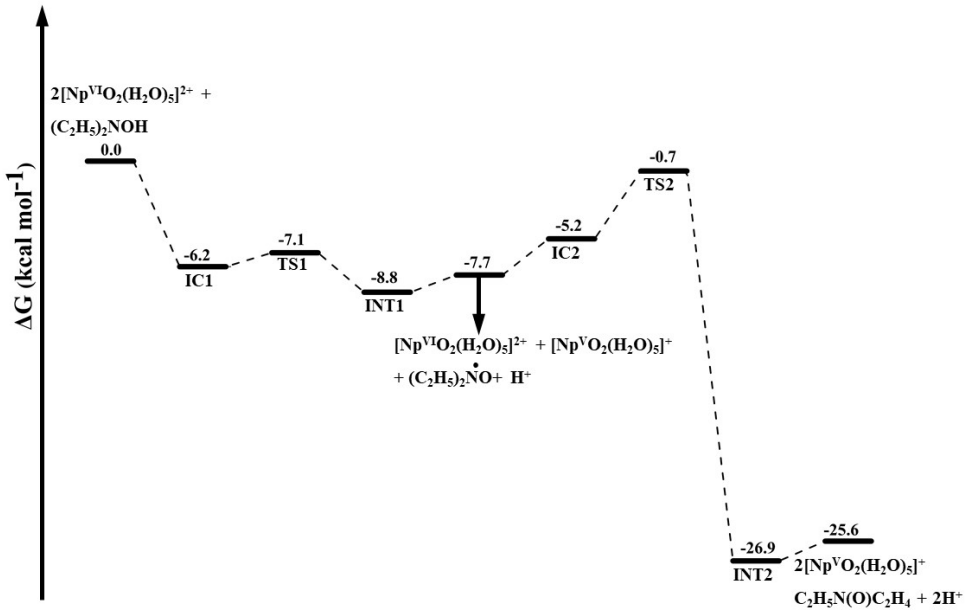

Fig. S1 Potential energy profiles at the first and second stages of the Np(VI) reduction by DEHA at the B3LYP/ECP60MWB/6-31G(d) level of theory.

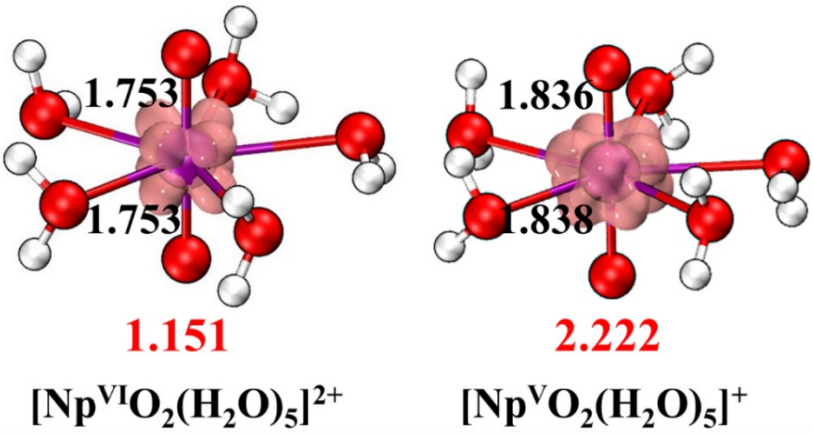

Fig. S2. The diagrams (isovalue = 0.02) of $[Np^{VI}O_2(H_2O)_5]^{2+}$ and $[Np^{V}O_2(H_2O)_5]^{+}$, and Np-O_{yl} bond distances (Å), values of the spin density on the Np atoms at the B3LYP/ECP60MWB/6-31G(d) level of theory.

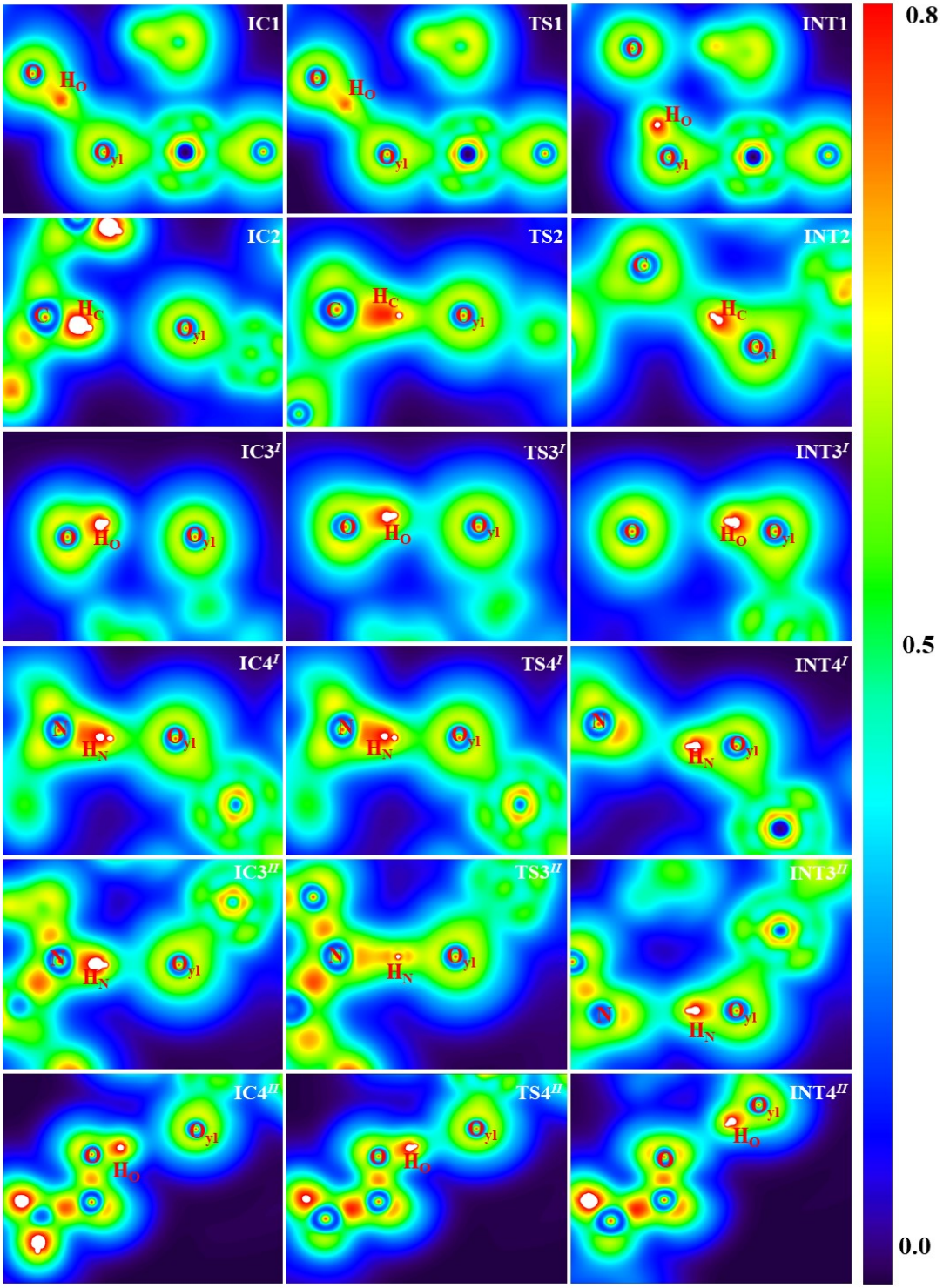

Fig. S3. Diagrams of LOL on the O_{yl}-H-C/N/O plane for the structures for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction with $(C_2H_5)_2NOH$. The range of the color scale for LOL is from 0 to 0.8.

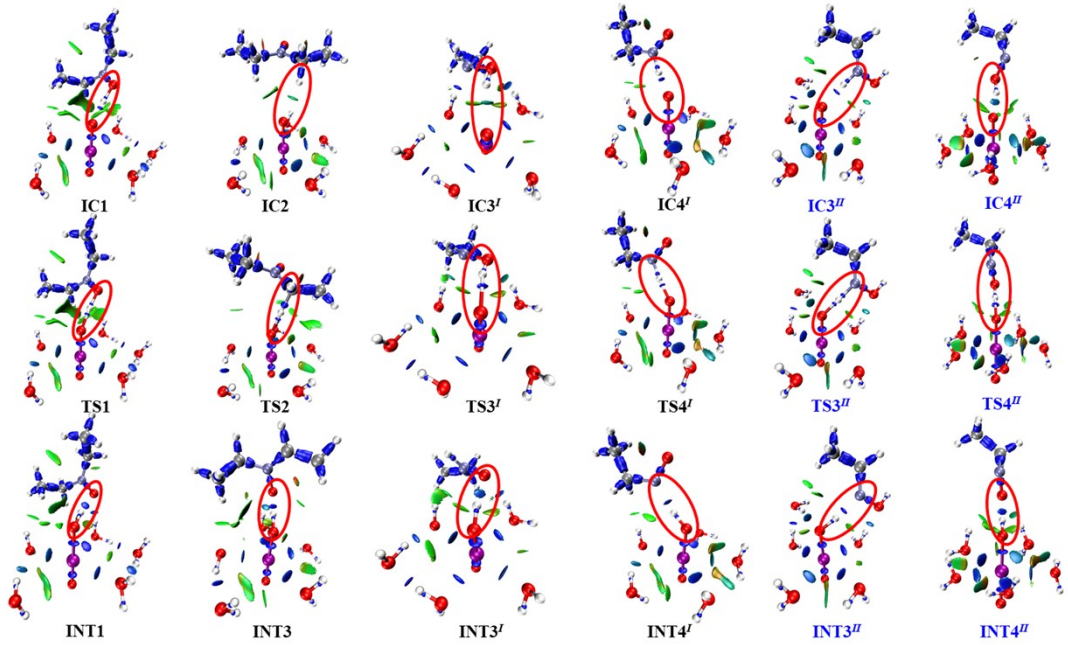

Fig. S4. IRI isosurfaces (IRI=1.0) images mapped by sign(λ_2)ρ corresponding to the structures of ICs, TSs and INTs for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction with $(C_2H_5)_2NOH$.

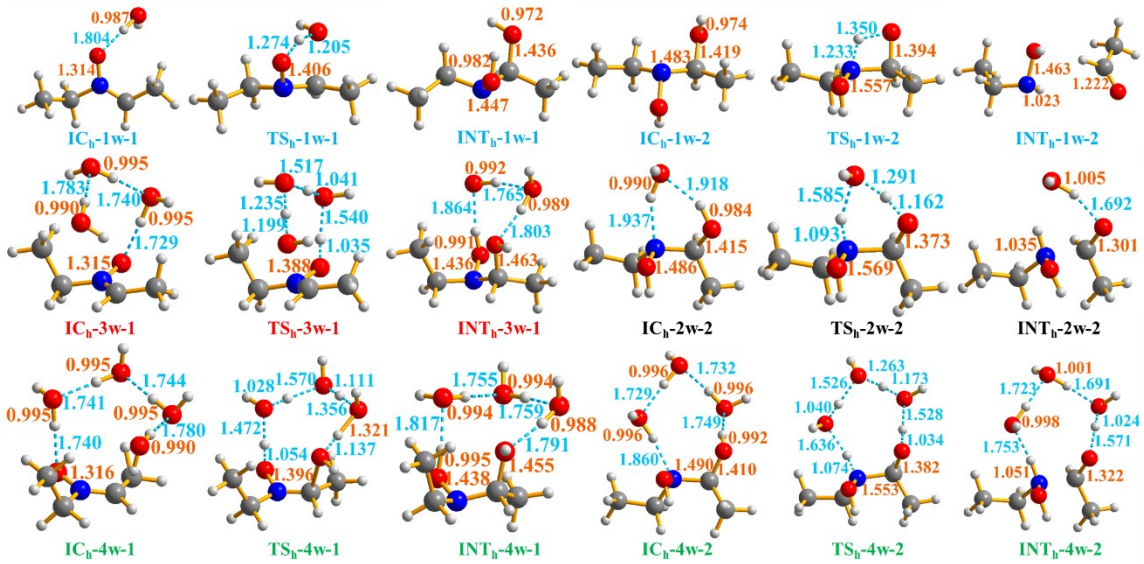

Fig. S5. The structures and the related bond distances (Å) of ICs, TSs, and INTs for the hydrolysis of $C_2H_5N(O)C_2H_4$ with n=1-4 water molecules at the B3LYP/6-31G(d) level of theory in the aqueous phase.

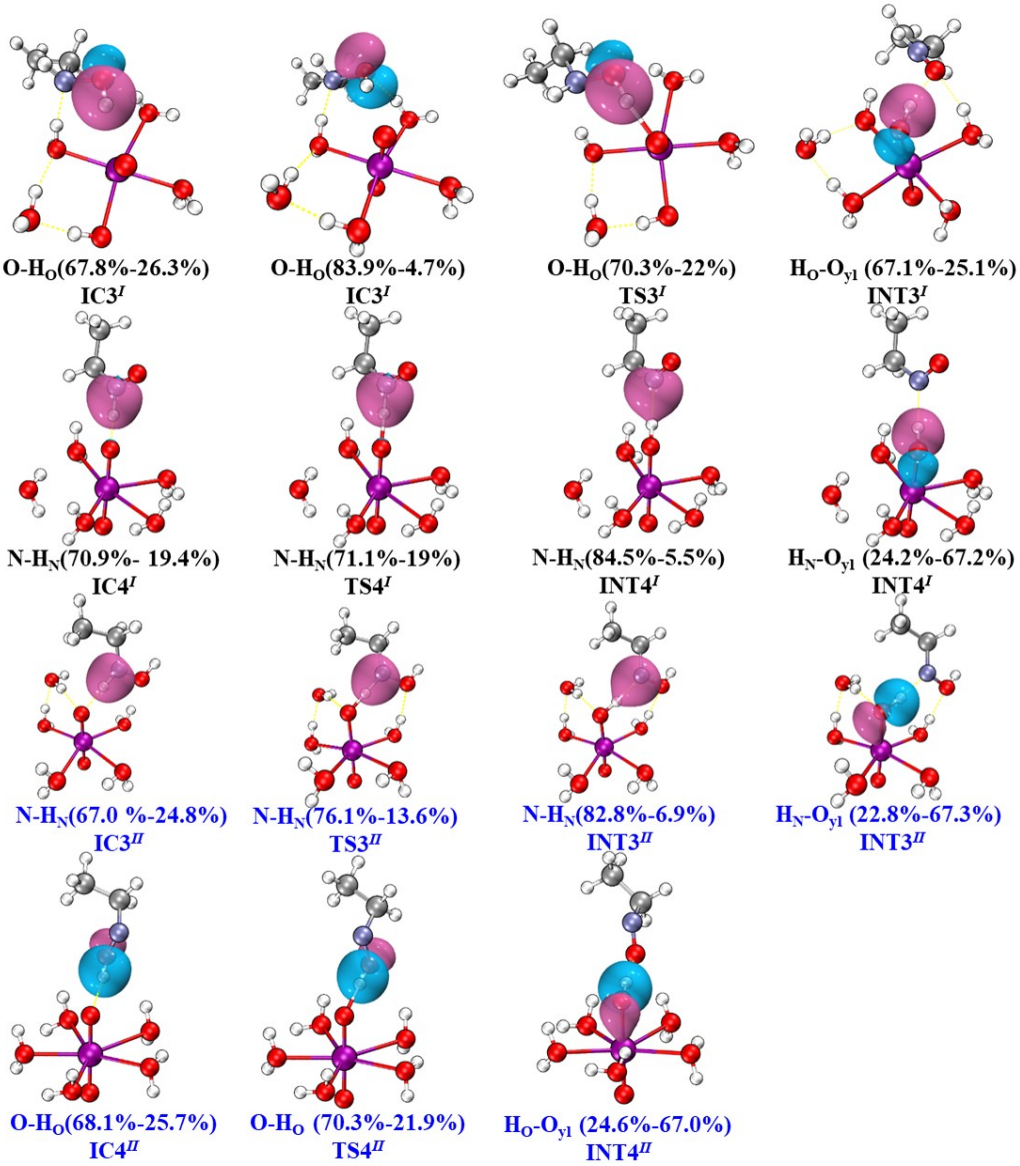

Fig. S6. Diagrams of LMOs (isovalue = 0.05) and the percentage of atoms of LMOs a for the structures of ICs, TSs, and INTs at the 3rd and 4th stages of $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction with $(C_2H_5)_2NOH$.

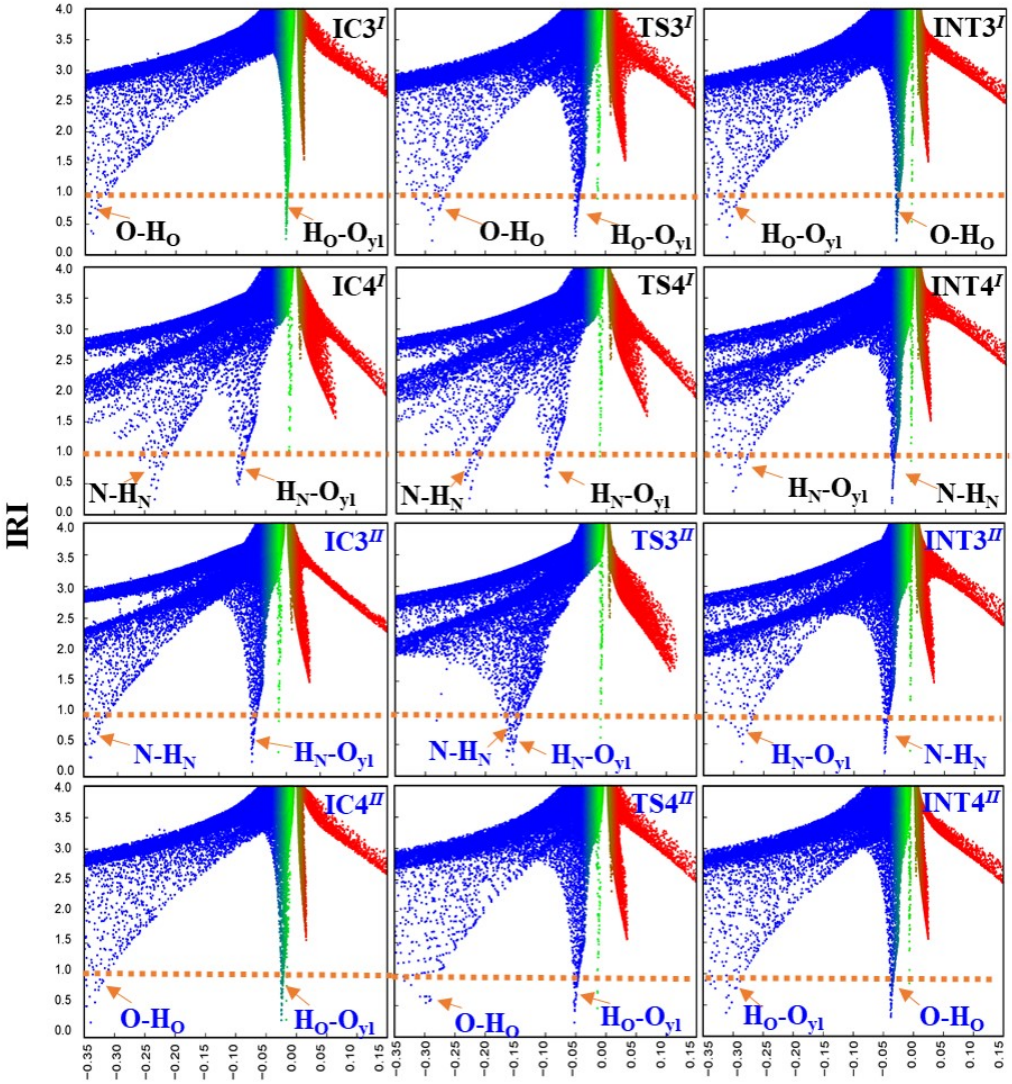

Fig. S7. Color-filled scatter maps between IRI and sign(λ_2)ρ of the structures for ICs, TSs, and INTs at the 3rd and 4th stages of $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction with $(C_2H_5)_2NOH$.

Cartesian coordinates

IC1

Atom	X	Y	Z (Angstrom)
Np	0.73387700	-0.07068000	0.00008000
O	1.55375900	2.02845500	1.33686000
H	1.13096300	2.13368400	2.20760600
O	2.14088200	-2.67016600	1.20311000
H	1.54659700	-2.84364600	0.44438300
O	0.31434500	-2.53489400	-0.98562800
H	-0.62506100	-2.77857000	-0.90922600
O	-0.41622900	1.60850000	-1.56390600
H	-1.30180500	1.72508500	-1.18017800
O	0.91943100	3.79863100	-0.71906300
H	0.20169900	4.37479700	-0.40395400
H	1.20663600	3.31606300	0.09014100
H	2.50964800	1.98728500	1.51935800
H	2.91201300	-2.25620100	0.78084000
H	0.52143500	-2.60686900	-1.93342700
H	0.06400000	2.45921300	-1.33902200
O	-0.86445200	-0.08893100	1.01162000
O	2.26230400	-0.05801600	-0.99114300
N	-3.87302200	0.41897400	-0.30809400
O	-3.07438900	0.93644800	0.60318500
H	-2.10779800	0.44149200	0.66798700
C	-5.25473600	0.89729900	-0.23490100
H	-5.73929900	0.57846700	-1.15872100
H	-5.20430800	1.99016200	-0.21792200
C	-3.41390700	-0.70071900	-1.13521900
H	-4.05143500	-0.70105600	-2.02086300
H	-2.39065900	-0.46526600	-1.43983000
C	-5.98993100	0.37035900	1.00070100
H	-5.47968900	0.67907700	1.91747800
H	-6.99951600	0.79294400	1.00396000
H	-6.06759000	-0.72043000	0.98156000
C	-3.47695900	-2.04753200	-0.40720400
H	-3.06914700	-2.81287600	-1.07646600
H	-2.87886800	-2.02760300	0.50776200
H	-4.50747300	-2.31601900	-0.15854600

TS1

Atom	X	Y	Z (Angstrom)
Np	1.14856600	-0.10550200	0.03554900
O	1.96240300	1.99730600	1.36332000
H	1.54637400	2.09447300	2.23826600
O	2.57616400	-2.69650100	1.22854900
H	1.97934300	-2.87356700	0.47271400
O	0.74470200	-2.56995200	-0.96028000
H	-0.19174200	-2.82766600	-0.89766500
O	-0.04480700	1.52258100	-1.54512500
H	-0.93804400	1.61430300	-1.17177700
O	1.22695700	3.74528900	-0.68398800
H	0.49502900	4.29338500	-0.35195300
H	1.54659200	3.26966200	0.11696400
H	2.92082800	1.97736300	1.53545000
H	3.33785900	-2.26814000	0.80336000
H	0.96294000	-2.62594000	-1.90671100
H	0.40810400	2.38737700	-1.31623400
O	-0.45413100	-0.13141100	1.05275100
O	2.67417000	-0.08703400	-0.95743400
N	-3.47556600	0.31613900	-0.21731700
O	-2.67216900	0.83373000	0.68705600
H	-1.66970000	0.35778200	0.73554600
C	-4.87141700	0.74209800	-0.09863100
H	-5.36213900	0.45496500	-1.03000000
H	-4.85711200	1.83348400	-0.02547800
C	-3.00694000	-0.77238200	-1.08034700
H	-3.66288300	-0.76769700	-1.95255500
H	-1.99672300	-0.50528500	-1.40157500
C	-5.56745300	0.12738200	1.11888100
H	-5.04816200	0.40099500	2.04184700
H	-6.58895300	0.51779700	1.16440600
H	-5.61349000	-0.96267800	1.04202500
C	-3.02196700	-2.13772800	-0.38553400
H	-2.61310700	-2.87726100	-1.08279400
H	-2.40284600	-2.12625100	0.51559900
H	-4.03952500	-2.43670200	-0.11927200

INT1

Atom	X	Y	Z (Angstrom)
Np	0.94450500	-0.12656800	0.17516000
O	1.72506400	1.99470400	1.44581900
H	1.31833000	2.07606300	2.32711800
O	2.36557200	-2.69034300	1.42055700
H	1.80095600	-2.88193500	0.64473900
O	0.55138400	-2.57960500	-0.81536100
H	-0.39450100	-2.80251300	-0.75323200
O	-0.20208700	1.37192700	-1.52109100
H	-1.14259200	1.32828100	-1.22388100
O	0.74748400	3.72420100	-0.56244600
H	-0.05238700	4.14234100	-0.19989100
H	1.14746500	3.27135500	0.21319000
H	2.68659800	2.01735200	1.60042300
H	3.17566200	-2.33562900	1.01754400
H	0.75834300	-2.60417900	-1.76601500
H	0.11665400	2.28270300	-1.25523600
O	-0.79202100	-0.12554800	1.20704600
O	2.46878200	-0.13732300	-0.79087100
N	-3.68067600	0.46037700	-0.91684000
O	-2.72975300	1.10469800	-0.31475700
H	-1.53353200	0.23399000	0.63922600
C	-5.05649600	0.78615400	-0.51897200
H	-5.72305000	0.24204800	-1.19102600
H	-5.18866800	1.85924500	-0.69343500
C	-3.34462800	-0.73650300	-1.69687500
H	-4.12533900	-0.86033700	-2.45191100
H	-2.40253700	-0.51583800	-2.20528000
C	-5.34417600	0.44983700	0.94526500
H	-4.65144600	0.98043600	1.60542800
H	-6.36389400	0.76486200	1.18983400
H	-5.25948100	-0.62515900	1.13234600
C	-3.21783300	-1.99851600	-0.83799700
H	-2.90969500	-2.83299500	-1.47762800
H	-2.46595400	-1.86169700	-0.05470700
H	-4.17133600	-2.26049500	-0.36906200

IC2

Atom	X	Y	Z (Angstrom)
Np	1.26974900	-0.04593700	0.10656700
O	2.24901800	2.47954500	-1.68068800
H	2.94629500	1.88536800	-1.34949900
O	2.15991200	-1.21988900	-2.13301400
H	2.82099200	-1.86079600	-1.81781200
O	0.91678600	-2.65187200	0.47977900
H	1.56889300	-2.85518700	1.17346600
O	0.25940300	-0.42665200	2.56409800
H	0.72660200	-1.22865700	2.85765600
O	0.91772800	2.58230900	0.72762300
H	1.60222800	2.71982600	1.40483600
H	1.38871900	2.75613700	-0.12682300
H	1.63713900	1.87177800	-2.13237100
H	1.42078900	-1.77419500	-2.43852300
H	1.32162100	-3.00363500	-0.33367100
H	-0.64137600	-0.73875200	2.37025900
O	2.97392700	-0.05152700	0.78367300
O	-0.43634500	-0.03957600	-0.58753600
N	-4.21007900	0.01724200	-0.20801300
O	-4.95419900	-0.21470400	0.69861700
C	-3.59505400	-1.08646600	-0.97850100
H	-2.51252500	-0.91240800	-0.87321200
H	-3.84204200	-0.86788500	-2.02491600
C	-3.86898000	1.41802900	-0.56027000
H	-2.77234600	1.44463000	-0.52296900
H	-4.15011100	1.51208000	-1.61654800
C	-4.04653400	-2.45037500	-0.51449200
H	-5.12740200	-2.57491200	-0.62665900
H	-3.54456600	-3.19412300	-1.13979500
H	-3.77097800	-2.63007300	0.52853100
C	-4.53791100	2.42814400	0.34096200
H	-4.22660600	3.42269500	0.00937500
H	-5.62753400	2.36470300	0.27429300
H	-4.23285800	2.29780000	1.38310400

TS2

Atom	X	Y	Z (Angstrom)
Np	1.14994400	-0.00717200	0.10904700
O	2.16422300	2.53550100	-1.63884200
H	2.85721800	1.94233900	-1.29754000
O	1.92526700	-1.23462100	-2.03965900
H	2.61098200	-1.88018500	-1.79339700
O	0.74826300	-2.59753100	0.49099100
H	1.36561000	-2.82015200	1.21031500
O	0.12789200	-0.38407200	2.55478600
H	0.53513200	-1.22091000	2.84024600
O	0.79829100	2.60282000	0.73618700
H	1.46663100	2.73847500	1.43017000
H	1.28313500	2.79757000	-0.10680000
H	1.56221500	1.92741600	-2.10285200
H	1.18282400	-1.77617300	-2.36011100
H	1.14655200	-3.00483600	-0.29897400
H	-0.79744400	-0.62339000	2.37094400
O	2.83973900	-0.02920100	0.78741100
O	-0.59918600	0.04604000	-0.66425700
N	-3.80464600	-0.15588200	-0.23592500
O	-4.19411100	-0.51381500	0.87504800
C	-2.98567800	-0.94603600	-1.01710900
H	-1.81574300	-0.43490900	-0.78398900
H	-3.08633100	-0.67437500	-2.06982100
C	-4.16323900	1.21762700	-0.72018500
H	-3.28137200	1.59155100	-1.24514300
H	-4.95356500	1.05668500	-1.46145400
C	-2.91183300	-2.40736400	-0.65505600
H	-3.90155500	-2.87655000	-0.71867400
H	-2.24153200	-2.90972300	-1.35694500
H	-2.52892200	-2.55112100	0.35933000
C	-4.61069100	2.12869800	0.40348800
H	-4.82740600	3.10991600	-0.02977300
H	-5.51717200	1.75843000	0.88807300
H	-3.82591700	2.24965000	1.15633800

INT2

Atom	X	Y	Z (Angstrom)
Np	1.10460600	-0.09439600	0.10899100
O	2.54358300	2.24439100	-1.60592900
H	3.13758600	1.60996300	-1.16466100
O	1.94728400	-1.40437400	-1.96764300
H	2.67848700	-1.95130400	-1.62687000
O	0.70608200	-2.61572900	0.70608400
H	1.12087400	-2.70316100	1.58335800
O	-0.31465000	-0.08472400	2.29015300
H	-0.26778900	-0.99150400	2.64214800
O	0.77805800	2.47584600	0.46129600
H	1.24867000	2.68429000	1.28756600
H	1.44229500	2.64853300	-0.25811100
H	1.94415800	1.66934500	-2.11428200
H	1.24235400	-2.04692000	-2.16551000
H	1.32525600	-3.06135200	0.09976200
H	-1.22758200	-0.00956300	1.93127800
O	2.76170600	-0.10032500	0.84146400
O	-0.62519200	-0.09346100	-0.89152700
N	-3.74797900	0.06588400	0.07817900
O	-2.64297200	-0.36235400	0.68103800
C	-4.42921900	-0.70775600	-0.70457700
H	-1.44468200	-0.20355600	-0.27332200
H	-5.30974400	-0.27079900	-1.16105900
C	-4.10888600	1.48421600	0.30970700
H	-5.11645400	1.63072000	-0.08343700
H	-4.12820500	1.61764900	1.39401900
C	-4.02035400	-2.11021900	-0.96662700
H	-3.91091800	-2.66270900	-0.02551000
H	-4.75845100	-2.60822800	-1.59761000
H	-3.04475000	-2.13660700	-1.46928000
C	-3.11346800	2.43177200	-0.34937800
H	-3.44006800	3.46149500	-0.17237500
H	-2.11032600	2.31360800	0.06743800
H	-3.07286100	2.26546700	-1.43122600

IC3^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.75165100	-0.17587400	-0.12824100
O	-2.55953200	-1.95214900	0.26522100
H	-3.01107800	-1.71499100	1.09564300
O	-2.52082200	1.62684200	0.25306900
H	-1.89910600	2.41015100	0.37000000
O	-0.65423900	3.53471200	0.50629500
H	-0.48823200	3.58821100	1.46323200
O	1.08060400	1.56936800	-0.49575500
H	1.87756000	1.14763700	-0.01802400
O	0.63831300	-2.35007000	-0.15131200
H	1.38430900	-2.00779500	0.40002700
H	0.14752800	-2.94681100	0.44279500
H	-3.23238800	-1.82269300	-0.42803400
H	-2.92255500	1.76038400	-0.62433600
H	0.06867700	2.95697600	0.17017000
H	1.31238000	1.59353100	-1.44145600
O	-0.45233200	-0.14026300	1.60454600
O	-1.06323900	-0.19731900	-1.84969000
N	3.06310100	0.17410100	0.75619500
H	3.68820700	0.60627800	1.44097200
O	2.39811000	-0.87743400	1.51047400
H	1.55638900	-0.46658800	1.79218400
C	3.90078600	-0.49510200	-0.25385400
H	3.22956300	-0.96527100	-0.97889700
H	4.49812200	-1.28439900	0.22083100
C	4.80142800	0.53147800	-0.92961200
H	5.47147000	1.00806400	-0.20445600
H	5.41901800	0.03497100	-1.68456900
H	4.21379700	1.31214900	-1.42505200

TS3^{I}

Atom	X	Y	Z (Angstrom)
Np	0.75768700	-0.16640500	0.11559500
O	2.58029100	-1.95912800	-0.34457500
H	2.68508900	-2.01476000	-1.31126400
O	2.55503000	1.63975400	-0.31102100
H	1.93727500	2.42139000	-0.41206800
O	0.67905200	3.57337300	-0.54667200
H	0.49252300	3.59521100	-1.50092100
O	-1.04119800	1.65603300	0.59977900
H	-1.90745300	1.33017900	0.28143600
O	-0.45133800	-2.51846900	0.33705400
H	-1.29619900	-2.27473800	-0.09034000
H	0.01886300	-3.02816700	-0.34687500
H	3.41756400	-1.56944100	-0.03585600
H	2.96587900	1.76126200	0.56227300
H	-0.04021400	3.01443600	-0.17741500
H	-1.15384700	1.78277800	1.55950700
O	0.12169600	-0.12965900	-1.61468800
O	1.30756200	-0.19834700	1.82946700
N	-3.15975300	-0.00181500	-0.76512100
H	-3.34519000	0.75495700	-1.43240100
O	-2.34344500	-0.95717500	-1.25967000
H	-1.47551200	-0.51847300	-1.57273300
C	-4.25231900	-0.49053800	0.06043900
H	-3.84817500	-1.31361400	0.65497700
H	-5.04014700	-0.89183100	-0.59353600
C	-4.78672600	0.63477000	0.94053000
H	-5.15900100	1.47115300	0.33994800
H	-5.61657400	0.24934900	1.54024500
H	-4.00841400	1.00222200	1.61734500

INT3^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.75711400	-0.18576600	-0.13575400
O	-2.55674800	-1.99986100	0.29796400
H	-2.78586900	-1.94465800	1.24301900
O	-2.56418300	1.60171700	0.25771100
H	-1.96489800	2.39432800	0.39185400
O	-0.72910200	3.54090000	0.59181000
H	-0.54176800	3.47080400	1.54390900
O	1.01978800	1.65830500	-0.56780300
H	1.85185800	1.52635300	-0.08025100
O	0.64829100	-2.37397300	-0.15145700
H	1.41666000	-2.01221800	0.35503500
H	0.20677400	-2.98215300	0.46756700
H	-3.35877300	-1.69653900	-0.16339500
H	-2.97922000	1.74420600	-0.61071200
H	-0.01963000	3.00225600	0.17378700
H	1.28051700	1.77820300	-1.49843400
O	-0.15189400	0.03842900	1.80324900
O	-1.27615800	-0.27319500	-1.86732600
N	3.34217100	-0.13807300	0.88278800
H	3.73916900	0.57605900	1.49974000
O	2.45666600	-0.91975500	1.40271900
H	0.80568000	-0.22227700	1.85063000
C	4.05152900	-0.49550000	-0.34594000
H	3.32844200	-1.00857600	-0.98541100
H	4.84702000	-1.20918800	-0.09245100
C	4.62821200	0.74418600	-1.01961700
H	5.30397100	1.28444600	-0.34715800
H	5.20020400	0.44202700	-1.90206600
H	3.83450900	1.42700300	-1.34160500

IC4^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.80756900	0.02342000	-0.10447600
O	-2.19867400	-0.02172000	2.10038500
H	-1.64687800	0.12540500	2.88807300
O	-0.85653600	3.04898800	0.83900700
H	-0.24928400	2.87053500	0.09064100
O	0.68424000	1.89866400	-1.26248200
H	1.65097900	1.88670700	-1.16693500
O	-0.41045200	-1.77598400	-1.94128900
H	-1.01357400	-2.44452200	-1.56611200
O	-2.21156600	-2.36812200	0.44205500
H	-1.47654400	-2.92612900	0.75148800
H	-2.47344800	-1.86819800	1.24169200
H	-2.87180100	0.68036000	2.12595000
H	-1.71498300	2.75975700	0.48527000
H	0.51419200	2.12994700	-2.19165000
H	-0.88736600	-1.44390800	-2.72289600
O	0.73794600	-0.54897600	0.82697400
O	-2.29309600	0.59459000	-0.99208000
N	3.25419100	-0.62444800	0.43882200
H	2.10754900	-0.54079000	0.53853100
O	3.76264300	-1.67392300	0.71044700
C	4.05083600	0.52390300	0.02556200
H	3.70028000	1.33913600	0.67605400
H	3.65960200	0.76497000	-0.97601600
C	5.54214800	0.29117900	0.05757000
H	5.83599700	-0.50103100	-0.63678700
H	6.03933200	1.21811500	-0.24035700
H	5.87656200	0.02407500	1.06460800

TS4^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.80704100	0.02343200	-0.10460700
O	-2.19636100	-0.02125900	2.10049800
H	-1.64353900	0.12643000	2.88737900
O	-0.85633800	3.04902100	0.83844800
H	-0.24941300	2.87084200	0.08976700
O	0.68412100	1.89839500	-1.26321000
H	1.65084700	1.88691800	-1.16761200
O	-0.41005000	-1.77619700	-1.94068400
H	-1.01243400	-2.44530400	-1.56531200
O	-2.21045200	-2.36797900	0.44259800
H	-1.47565200	-2.92602000	0.75252800
H	-2.47297700	-1.86823200	1.24211700
H	-2.86876800	0.68153800	2.12582100
H	-1.71492400	2.75977700	0.48506500
H	0.51400900	2.12756100	-2.19290000
H	-0.88717900	-1.44496900	-2.72252700
O	0.74163600	-0.54847200	0.82689100
O	-2.29333800	0.59365700	-0.99074300
N	3.24965800	-0.62409000	0.43869300
H	2.09501800	-0.54073200	0.54050500
O	3.75979600	-1.67313000	0.71024700
C	4.04777500	0.52362000	0.02526800
H	3.69746300	1.33957500	0.67487200
H	3.65782200	0.76427700	-0.97684000
C	5.53916000	0.29072800	0.05834600
H	5.83337300	-0.50210900	-0.63514900
H	6.03690800	1.21726300	-0.23997100
H	5.87296200	0.02427200	1.06576600

INT4^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.85325800	0.02626800	-0.10019000
O	-2.24610900	0.03220000	2.09139800
H	-1.62656100	0.08566300	2.84065300
O	-0.86561400	3.06746000	0.78545600
H	-0.23262400	2.87131600	0.06666800
O	0.68171600	1.77722600	-1.26386600
H	1.62049300	1.53687700	-1.16359300
O	-0.44522700	-1.78889900	-1.90074900
H	-1.03621300	-2.46479800	-1.51790700
O	-2.29064000	-2.33205400	0.40684300
H	-1.59353300	-2.88563800	0.80046800
H	-2.66653700	-1.85773800	1.17345500
H	-2.73927900	0.87180700	2.11602400
H	-1.71676400	2.82256700	0.38385400
H	0.52805200	1.82616400	-2.22404500
H	-0.92609200	-1.47284800	-2.68694000
O	0.65131700	-0.72816200	1.00917700
O	-2.24887400	0.67577000	-1.04194400
N	3.41894800	-0.62054200	0.38173200
H	1.57751000	-0.61238100	0.64285600
O	4.03958100	-1.61842900	0.67929100
C	4.23237600	0.54357800	-0.01656200
H	3.86916700	1.35536400	0.62919700
H	3.86398800	0.78883800	-1.02432400
C	5.73323500	0.35225700	0.04258600
H	6.05838100	-0.45414200	-0.62193300
H	6.22533300	1.27795000	-0.26983600
H	6.05991000	0.11359300	1.05986700

IC3^{II}

Atom	X	Y	Z (Angstrom)
Np	0.77745400	-0.06908100	0.07466500
O	-1.50614000	2.68930600	0.90288400
H	-1.40713200	1.92427300	0.29108700
O	-0.42975300	-1.85310400	1.58651200
H	-1.38727700	-1.85887200	1.40599800
O	0.78536700	-2.24998200	-1.42730100
H	1.17290500	-1.74809400	-2.17105700
O	1.81010800	0.28963300	-2.39335800
H	1.27464300	0.99776700	-2.79126200
O	1.19309100	2.35926700	1.05846200
H	0.23991100	2.62750100	1.13326200
H	1.49310200	2.22091200	1.97300000
H	-1.85245600	2.28606600	1.71781400
H	-0.35423700	-1.58441700	2.51859500
H	1.52775500	-2.78179500	-1.09083700
H	2.69237900	0.68473200	-2.28046600
O	-0.84235300	0.42387500	-0.74809200
O	2.35673200	-0.52101300	0.87146300
N	-3.33086100	-0.47033700	-0.20270900
H	-2.37185300	-0.08369600	-0.44852800
O	-3.22268000	-1.64583700	0.39578400
H	-4.11628100	-1.97606800	0.64938800
C	-4.62079300	0.16151900	-0.41904100
H	-5.15637200	0.13502200	0.53842000
H	-5.17523100	-0.46810600	-1.12804000
C	-4.43858400	1.58021400	-0.93731700
H	-3.92227900	1.58684300	-1.90190900
H	-5.42873900	2.02371700	-1.07345400
H	-3.87672200	2.19201700	-0.22633900

TS3*II*

Atom	X	Y	Z (Angstrom)
Np	0.86673600	-0.18134500	0.05328600
O	-1.28721700	2.62052700	1.11054700
H	-1.32606000	1.91119200	0.43536400
O	-0.36213000	-1.94484500	1.55476600
H	-1.27418900	-2.00447700	1.20829400
O	0.86855200	-2.36656500	-1.41491900
H	1.24521300	-1.88927600	-2.17973100
O	1.90052500	0.17545100	-2.40835400
H	1.46790500	0.97389600	-2.75820100
O	1.38172700	2.16930700	1.01330600
H	0.44740700	2.46976600	1.17800700
H	1.77266600	2.03588700	1.89395100
H	-1.59655100	2.18269500	1.92236300
H	-0.46268200	-1.59153400	2.45608800
H	1.60865100	-2.90454900	-1.08286100
H	2.82970200	0.43537200	-2.28102300
O	-0.78748300	0.38361600	-0.80899200
O	2.43464600	-0.64990900	0.84014200
N	-3.05041200	-0.53868700	-0.33354000
H	-1.88229000	-0.07060500	-0.59151100
O	-2.97935900	-1.78157800	0.17120800
H	-3.86791100	-2.07963500	0.47083200
C	-4.36283100	0.08127400	-0.36964200
H	-4.82581300	-0.04701100	0.61907400
H	-4.97719300	-0.47270700	-1.09393700
C	-4.24990100	1.55241500	-0.74722400
H	-3.79677600	1.67429500	-1.73609000
H	-5.25302300	1.98798700	-0.77414600
H	-3.65337600	2.10387700	-0.01484700

INT3^{II}

Atom	X	Y	Z (Angstrom)
Np	0.76884700	-0.04622100	0.04425500
O	-1.41364600	2.91266200	0.68021300
H	-1.39389100	2.14084000	0.07205700
O	-0.46522900	-1.65382100	1.62017000
H	-1.40444800	-1.74202000	1.34732100
O	0.77174500	-2.24471100	-1.33367100
H	1.25943100	-1.87358400	-2.09431800
O	1.80216600	0.32569800	-2.40620400
H	1.25692800	1.03300000	-2.79344000
O	1.23572700	2.32202400	0.99088100
H	0.30284900	2.67086200	0.99563800
H	1.47915100	2.22077100	1.92763300
H	-1.83481900	2.55919300	1.48282700
H	-0.49486700	-1.27835400	2.51783400
H	1.41281800	-2.83566600	-0.89981300
H	2.67250900	0.73974300	-2.26675500
O	-0.93531100	0.55769500	-0.88728700
O	2.33512600	-0.48469300	0.82954500
N	-3.28923600	-0.63406500	-0.12454100
H	-1.77920000	0.05524600	-0.63708700
O	-3.12221400	-1.80316900	0.56173300
H	-3.93970300	-2.03969600	1.05456900
C	-4.63252900	-0.09409200	-0.00336700
H	-4.89449800	-0.02845000	1.06401200
H	-5.33787900	-0.80045900	-0.46737100
C	-4.70596100	1.27427800	-0.66935800
H	-4.47262900	1.20566400	-1.73705700
H	-5.71780900	1.67803200	-0.56621100
H	-4.00574900	1.97617000	-0.20386700

IC4^{II}

Atom	X	Y	Z (Angstrom)
Np	-0.95742600	-0.01607200	0.05685200
O	0.36133300	2.10535400	1.33697700
H	0.16973300	1.96905200	2.28130600
O	0.52917400	-1.17144600	1.82235300
H	0.06376400	-2.00509700	2.02011300
O	-1.26721100	-2.55650900	-0.26501500
H	-0.36889200	-2.92097800	-0.16212000
O	-2.70360100	-0.38533300	-1.80260400
H	-2.94685300	-1.32182900	-1.68209000
O	-1.33620100	2.44517600	-0.90774200
H	-2.23585600	2.67191900	-0.61062100
H	-0.75493700	2.81624300	-0.21073600
H	1.29301300	1.83970800	1.23584600
H	1.33968600	-1.45229200	1.36002400
H	-1.74553700	-2.86990900	0.52422900
H	-2.18772900	-0.37744700	-2.62959800
O	-2.33916400	0.04452800	1.12515400
O	0.42960500	-0.09419600	-1.01844100
N	3.84515800	0.61285700	-0.79758400
O	3.01808800	0.15060800	0.21201000
H	2.12247000	0.16069400	-0.18399000
C	5.20525000	0.44611600	-0.30859700
H	5.27848500	0.80782000	0.72568200
H	5.83413800	1.08223600	-0.93848000
C	5.68035700	-1.00964000	-0.39356500
H	5.62739100	-1.37756400	-1.42419600
H	6.71993300	-1.08311500	-0.05631800
H	5.06586500	-1.65902800	0.23824900

TS4^{II}

Atom	X	Y	Z (Angstrom)
Np	-0.93542000	-0.01655900	0.06714800
O	0.35964600	2.13618100	1.35001800
H	0.19354100	2.04072600	2.30350500
O	0.57437000	-1.20884500	1.84856600
H	0.27454300	-2.13423400	1.79611300
O	-1.33058100	-2.58674400	-0.22613500
H	-0.45332900	-2.99174600	-0.34801800
O	-2.70564800	-0.42448700	-1.78087000
H	-2.83709400	-1.38172500	-1.64592500
O	-1.32161900	2.45983400	-0.91003600
H	-2.23811700	2.66847500	-0.65713800
H	-0.78330400	2.81384000	-0.17141300
H	1.31749500	1.99911500	1.25090900
H	1.45658300	-1.22224500	1.43646200
H	-1.63932100	-2.93313400	0.63021300
H	-2.20358200	-0.37393600	-2.61411700
O	-2.32499900	0.11537400	1.18299100
O	0.47252900	-0.16945100	-1.07436300
N	3.72905200	0.08978500	-0.93360300
O	2.82528100	0.46207300	-0.07543000
H	1.91924700	0.20461300	-0.45767400
C	5.04034700	0.42941800	-0.43962800
H	4.97403200	1.12068800	0.40447600
H	5.56154800	0.90600600	-1.27896500
C	5.79294000	-0.86000600	-0.05868000
H	5.84609400	-1.55190500	-0.90389100
H	6.81033800	-0.58479400	0.23527600
H	5.30049900	-1.35621700	0.78255000

$INT4^{II}$

Atom	X	Y	Z (Angstrom)
Np	1.00409100	0.01534600	-0.10640500
O	-0.77155900	1.90015500	-1.06063200
H	-0.64228500	1.85814900	-2.02430600
O	-0.60493200	-1.24730300	-1.69041300
H	-0.38886100	-2.17646800	-1.48722800
O	1.54759600	-2.56250600	0.24052200
H	0.70941200	-2.97510400	0.51468500
O	2.81668800	-0.39439500	1.70766800
H	2.78920500	-1.36785700	1.62539500
O	1.35371100	2.49286100	0.84933800
H	2.13964000	2.81484500	0.37336000
H	0.60249100	2.80539400	0.30565600
H	-1.65612700	1.51631500	-0.91668400
H	-1.48720700	-1.11932700	-1.29792100
H	1.74284300	-2.95733300	-0.62781900
H	2.37272700	-0.21225500	2.55535200
O	2.27031000	0.27106700	-1.37642900
O	-0.38620500	-0.28248600	1.33382000
N	-3.92857300	0.02294300	0.84786300
O	-2.89449800	0.26464100	0.24449400
H	-1.30531900	-0.11852000	0.98758900
C	-5.14128600	0.39819800	0.11444700
H	-4.88178200	0.71441200	-0.89996200
H	-5.53275800	1.25828600	0.67672500
C	-6.15188400	-0.74646100	0.16469600
H	-6.37847100	-1.02732300	1.19774400
H	-7.07838300	-0.42141500	-0.31741200
H	-5.77540900	-1.62624400	-0.36638800