Theoretical study on the kinetic behavior of Np(VI) reduction with hydroxylamine and its derivatives: substituent effect

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Table S1 The change of Gibbs energy (ΔG, kcal mol^{-1}) for the reduction reactions of $[Np^{VI}O_2(H_2O)_5]^{2+}$ by HA, MHA and DMHA and its protonated forms at B3LYP/ECP60MWB/6-31G(d).

Reactions	ΔG(kcal mol^{-1})
$[Np^{VI}O_2(H_2O)_5]^{2+} + NH_2OH = [Np^{V}O_2(H_2O)_5]^{+} + NH_2O\bullet + H^{+}$	-3.5
$[Np^{VI}O_2(H_2O)_5]^{2+} + NH_3OH^{+} = [Np^{V}O_2(H_2O)_5]^{+} + NH_2O\bullet + 2H^{+}$	7.3
$[Np^{VI}O_2(H_2O)_5]^{2+} + CH_3NHOH = [Np^{V}O_2(H_2O)_5]^{+} + CH_3NHO\bullet + H^{+}$	-6.4
$[Np^{VI}O_2(H_2O)_5]^{2+} + CH_3NH_2OH^{+} = [Np^{V}O_2(H_2O)_5]^{+} + CH_3NHO\bullet + 2H^{+}$	6.0
$[Np^{VI}O_2(H_2O)_5]^{2+} + (CH_3)_2NOH = [Np^{V}O_2(H_2O)_5]^{+} + (CH_3)_2NO\bullet + H^{+}$	-6.9
$[Np^{VI}O_2(H_2O)_5]^{2+} + (CH_3)_2NHOH^{+} = [Np^{V}O_2(H_2O)_5]^{+} + (CH_3)_2NO\bullet + 2H^{+}$	5.7

Table S2. The values of $\rho(r)$, $\nabla^2\rho(r)$, $H(r)$, $G(r)$ and $V(r)$ (au) of the N/O-H and H-O$_{yl1}$ bonds for the structures of Np(VI) reduction with MHA at the B3LYP/ECP60MWB/6-31G(d) level of theory.

	Bond	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	$G(r)$	$V(r)$	$-G(r)/V(r)$
IC^{M}1	O-H$_O$	0.336	-1.818	-0.512	0.058	-0.570	0.101
	H$_O$-O$_{yl}$	0.024	0.082	0.000	0.020	-0.020	1.005
TS^{M}1	O-H$_O$	0.307	-1.594	-0.454	0.056	-0.510	0.109
	H$_O$-O$_{yl}$	0.043	0.137	-0.001	0.035	-0.037	0.970
INT^{M}1	O-H$_O$	0.042	0.128	-0.002	0.034	-0.035	0.953
	H$_O$-O$_{yl}$	0.300	-1.485	-0.431	0.060	-0.490	0.121
IC^{M}2	N-H$_N$	0.221	-0.866	-0.268	0.052	-0.320	0.162
	H$_N$-O$_{yl}$	0.100	0.166	-0.033	0.075	-0.107	0.694
TS^{M}2	N-H$_N$	0.218	-0.832	-0.261	0.053	-0.314	0.168
	H$_N$-O$_{yl}$	0.104	0.156	-0.037	0.076	-0.113	0.673
INT^{M}2	N-H$_N$	0.031	0.085	-0.001	0.022	-0.023	0.968
	H$_N$-O$_{yl}$	0.303	-1.509	-0.436	0.059	-0.495	0.119

Table S3. The values of $\rho(r)$, $\nabla^2\rho(r)$, $H(r)$, $G(r)$ and $V(r)$ (au) of the N/C-H and H-O_{yl1} bonds for the structures of Np(VI) reduction with DMHA at the B3LYP/ECP60MWB/6-31G(d) level of theory.

	Bond	$\rho(r)$	$\nabla^2\rho(r)$	$H(r)$	$G(r)$	$V(r)$	$-G(r)/V(r)$
IC^D1	O-H_O	0.337	-1.809	-0.510	0.058	-0.568	0.102
	H_O-O_{yl}	0.021	0.072	0.000	0.018	-0.018	1.008
TS^D1	O-H_O	0.308	-1.615	-0.459	0.055	-0.514	0.107
	H_O-O_{yl}	0.039	0.124	-0.001	0.032	-0.033	0.973
INT^D1	O-H_O	0.046	0.141	-0.002	0.037	-0.040	0.945
	H_O-O_{yl}	0.292	-1.412	-0.413	0.060	-0.474	0.127
IC^D2	C-H_C	0.263	-0.937	-0.263	0.029	-0.292	0.100
	H_C-O_{yl}	0.020	0.059	-0.000	0.015	-0.015	0.986
TS^D2	C-H_C	0.171	-0.353	-0.124	0.036	-0.161	0.226
	H_C-O_{yl}	0.106	0.151	-0.034	0.072	-0.107	0.678
INT^D2	C-H_C	-	-	-	-	-	-
	H_C-O_{yl}	0.290	-1.389	-0.407	0.060	-0.467	0.128
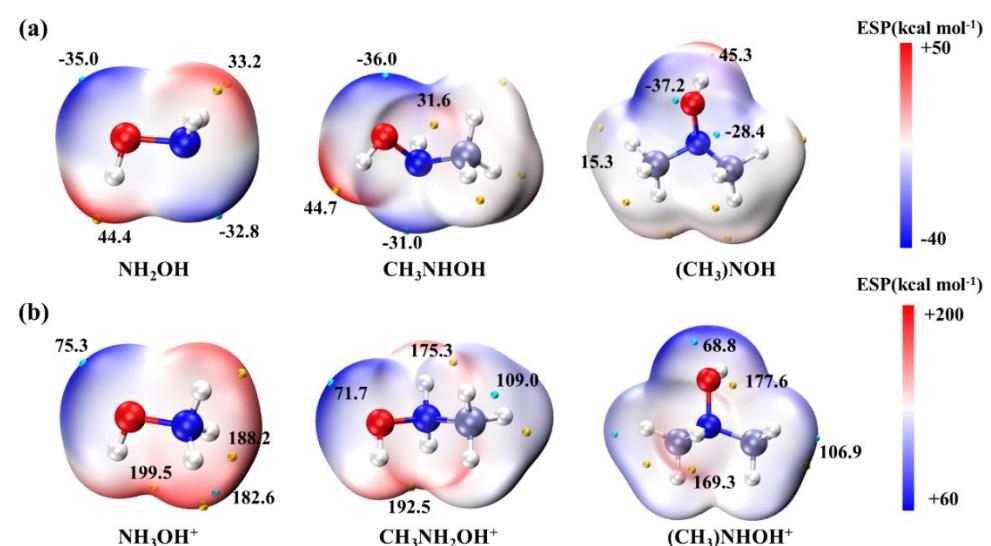
Figure S1 Electrostatic potential maps for HA, MHA, DMHA and the corresponding protonated forms.
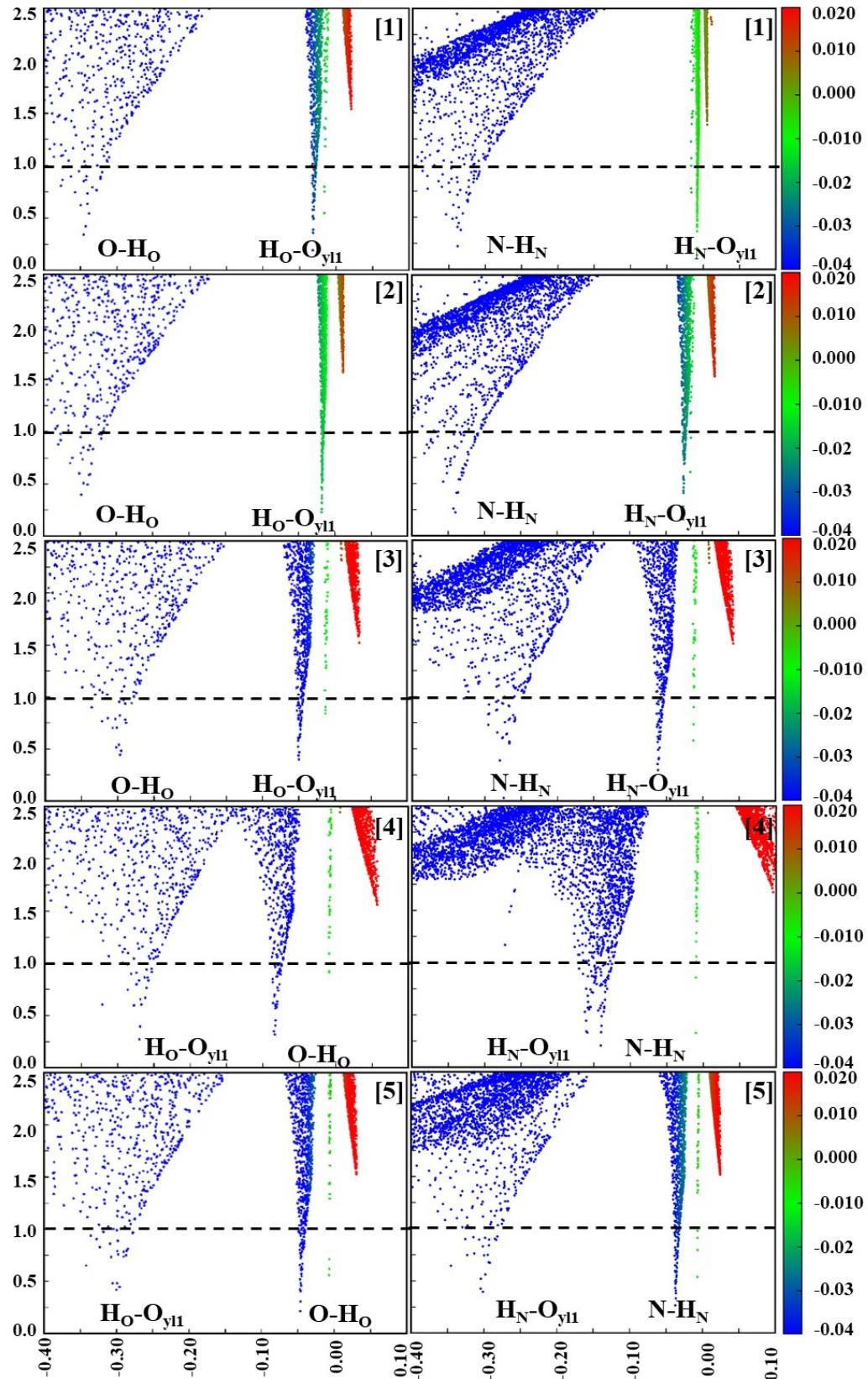
Figure S2. IRI scatter plots between IRI and sign(λ_2)ρ corresponding to the five points along the IRC for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction by HA.
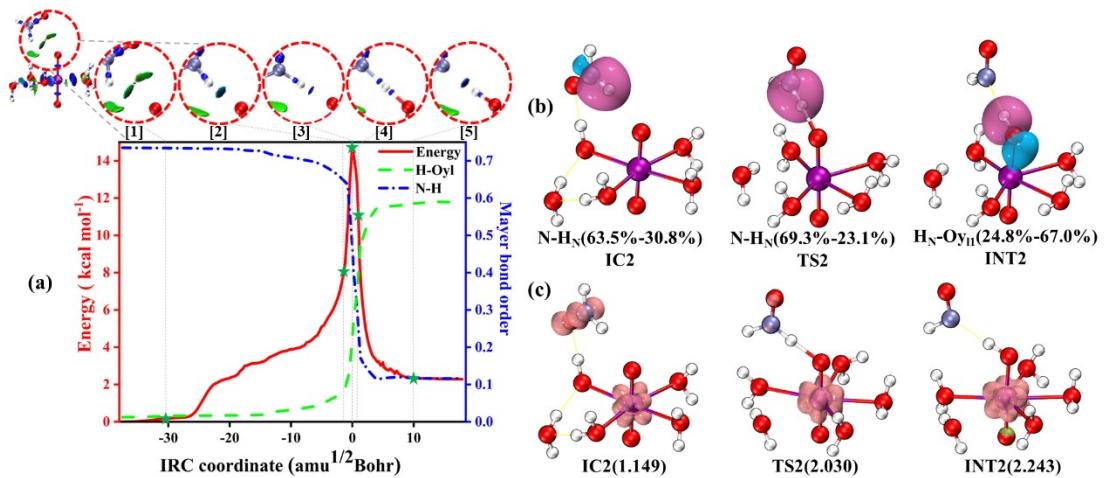
Figure S3. Mayer bond orders of the H_N-O_{yl1} and N-H_N bonds and color-filled IRI isosurface diagrams for the points along the IRC of TS2(a); LMO diagrams of IC2, TS2 and INT2(b); Spin density diagram of IC2, TS2 and INT2(c) for the second $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction by HA.
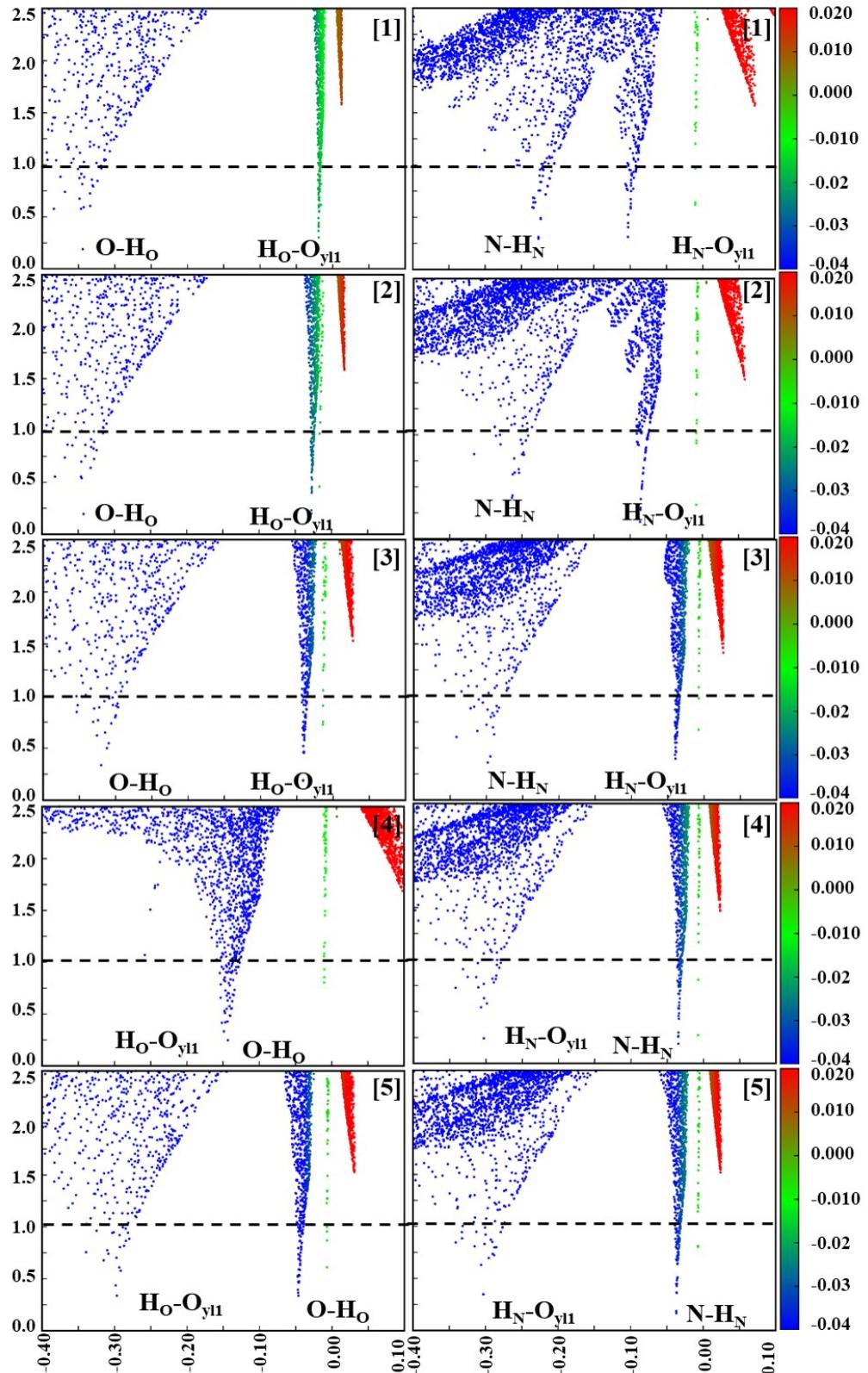
Figure S4. IRI scatter plots between IRI and sign(λ_2)ρ corresponding to the five points along the IRC for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction by MHA.
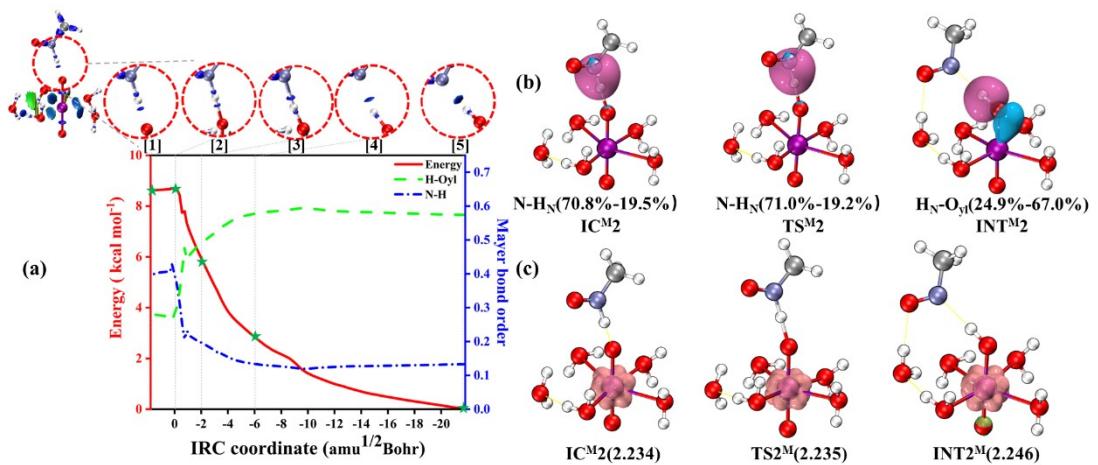
Figure S5. Mayer bond orders of the H_N-O_{yl1} and N-H_N bonds and color-filled IRI isosurface diagrams for the points along the IRC of TS^M2(a); LMO diagram of IC^M2, TS^M2 and INT^M2(b); Spin density diagram of IC^M2, TS^M2 and INT^M2(c) for the second Np(VI) reduction by MHA.
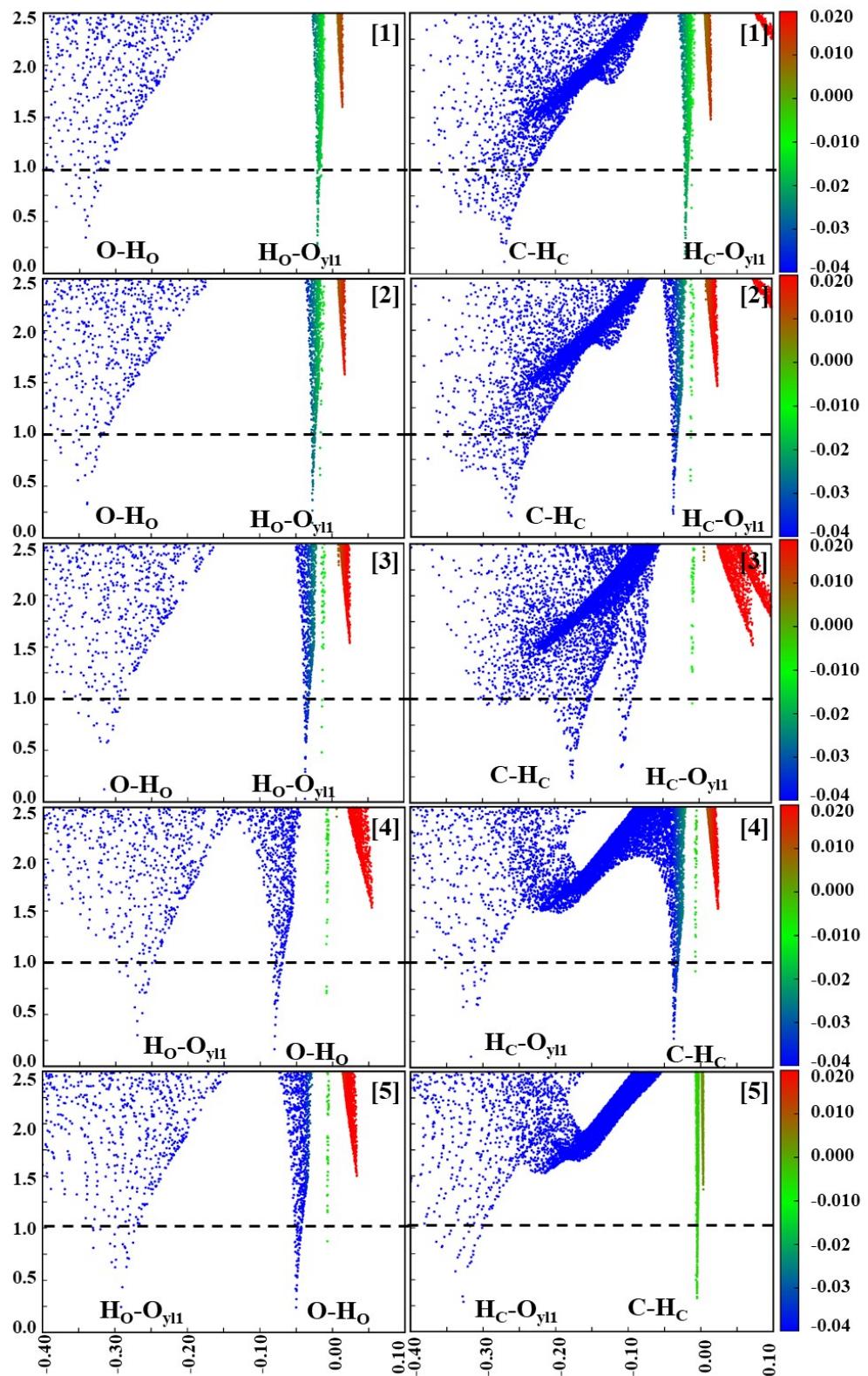
Figure S6. IRI scatter plots between IRI and sign(λ_2)ρ corresponding to the five points along the IRC for the $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction by DMHA.
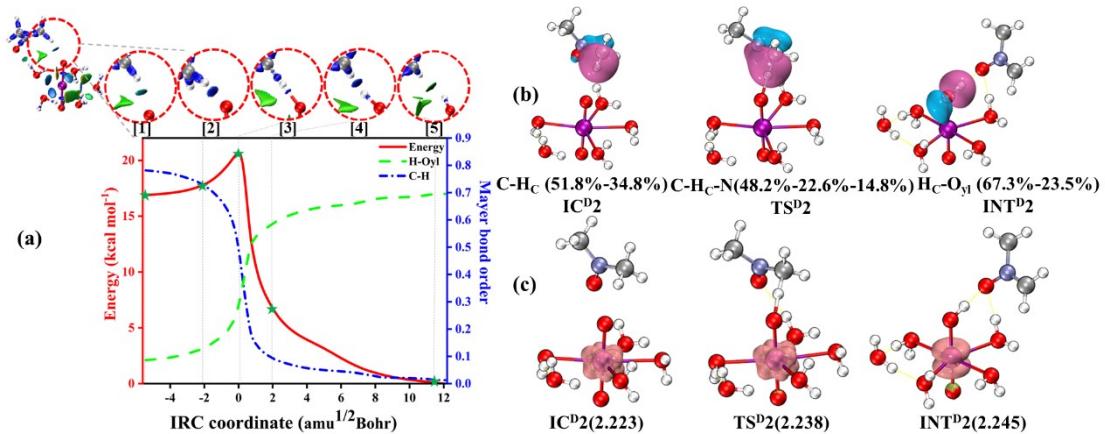
Figure S7. Mayer bond orders of the H_C-O_{yl1} and C-H_C bonds and color-filled IRI isosurface diagrams for the points along the IRC of TS^D2(a); LMO diagram of IC^D2, TS^D2 and INT^D2(b); Spin density diagram of IC^D2, TS^D2 and INT^D2(c) for second $[Np^{VI}O_2(H_2O)_5]^{2+}$ reduction by DMHA.

Cartesian coordinates

IC1

Atom	X	Y	Z (Angstrom)
Np	0.26920700	-0.31715400	0.05902200
O	-0.99305500	-2.40314300	-0.73614900
H	-1.15051000	-2.30271700	-1.69264000
O	2.45134400	-0.31677300	-1.25211700
H	2.77528000	0.61669700	-1.05904500
O	3.11107400	2.18325400	-0.55489200
H	2.70231800	2.74869000	-1.23291700
O	1.05786400	1.77403700	1.34143100
H	0.38747100	2.48119100	1.36100500
O	-1.91209100	-0.31578100	1.39304900
H	-2.42692800	0.39757300	0.92771300
H	-2.33221500	-1.15188400	1.11975800
H	-0.38804200	-3.16354200	-0.66191600
H	3.04808300	-0.89801200	-0.74779000
H	2.46402700	2.19576500	0.18523700
H	1.25527800	1.57601000	2.27502300
O	-0.45327800	0.70041400	-1.17945100
O	0.99500300	-1.32603500	1.29199700
N	-4.14510000	1.06410700	-0.86889700
O	-3.08706900	1.66544100	-0.06142700
H	-4.55639400	0.38482200	-0.22574400
H	-2.31977900	1.65724300	-0.66286900
H	-4.83750600	1.81342300	-0.93214600

TS1

Atom	X	Y	Z (Angstrom)
Np	0.30018000	-0.32553400	0.09468600
O	0.30665400	-2.52956300	-1.24068800
H	0.43641200	-2.30938400	-2.18040800
O	2.41361600	0.43435600	-1.15867900
H	2.35554800	1.41739300	-0.97410200
O	2.04025600	3.01690200	-0.47049500
H	1.45016900	3.36185100	-1.16248400
O	0.26677100	1.89765800	1.42210400
H	-0.60370000	2.33462700	1.40816900
O	-1.81294700	-1.10757200	1.39662500
H	-2.48754700	-0.48413600	1.06468300
H	-2.06372000	-1.96841400	1.01594700
H	1.10542000	-3.02729800	-0.99156900
H	3.16186300	0.12658900	-0.61816000
H	1.42795300	2.76315800	0.25586200
H	0.49382700	1.80102600	2.36414400
O	-0.75166700	0.45073100	-1.17939200
O	1.34603200	-1.08620800	1.33465400
N	-4.04473500	0.76233200	-0.90318200
O	-3.03876700	1.15313400	-0.07645000
H	-4.93709100	0.97934600	-0.46223300
H	-2.16695000	0.99164700	-0.56857100
H	-3.93538200	1.11642300	-1.85625700

INT1

Atom	X	Y	Z (Angstrom)
Np	0.31839800	-0.31304400	0.10321200
O	0.34175500	-2.52673500	-1.20733500
H	0.51833700	-2.33829100	-2.14594900
O	2.43429300	0.38884300	-1.15030100
H	2.40815400	1.37222200	-0.95722200
O	2.11436800	2.97220500	-0.47807900
H	1.55983600	3.31588900	-1.19966700
O	0.27299400	1.92009900	1.41163500
H	-0.59484100	2.36112500	1.37422000
O	-1.82011700	-1.02164000	1.37058200
H	-2.47355800	-0.41254200	0.95525200
H	-2.04756100	-1.90233100	1.02230200
H	1.10634100	-3.05265400	-0.91260300
H	3.17417100	0.04840500	-0.61749200
H	1.47031300	2.74494900	0.22929500
H	0.49257000	1.85805100	2.35810000
O	-0.79531900	0.47184300	-1.40408000
O	1.35785200	-1.05835000	1.38773800
N	-4.28607100	0.83993800	-0.74374600
O	-3.16091900	0.92947100	-0.12698400
H	-5.12830700	0.66963700	-0.19369900
H	-1.69328300	0.73277000	-1.04684600
H	-4.35995500	1.23039100	-1.68361300

IC2

Atom	X	Y	Z (Angstrom)
Np	-0.46997300	-0.04410300	-0.06612100
O	-0.30729700	1.93725300	1.44351400
H	0.22983800	1.65896900	2.20700500
O	1.35253800	3.20633600	-0.20722100
H	1.63843300	2.34800100	-0.59633800
O	1.77921300	0.56332800	-1.08165700
H	2.52465600	-0.02652600	-0.76631500
O	-1.16488200	-2.14794700	-1.33373500
H	-1.30275600	-2.85502100	-0.67802700
O	-2.62845500	-0.71871900	1.17040900
H	-2.38046600	-0.84077200	2.10469400
H	-3.22028200	0.05559800	1.17068200
H	0.30164300	2.52027800	0.88991400
H	0.76126900	3.58236200	-0.88239200
H	1.75818900	0.48799100	-2.05249700
H	-2.04442300	-1.99304200	-1.72299500
O	0.33448400	-1.03334600	1.14501200
O	-1.26423900	0.93988100	-1.27905300
N	3.42831200	-1.56175100	0.93298300
O	3.76512900	-1.01216000	-0.18377500
H	4.06254900	-2.25160600	1.33479700
H	2.44874400	-1.52939600	1.22191900

TS2

Atom	X	Y	Z (Angstrom)
Np	-0.41918700	0.00771400	-0.12132300
O	-1.52382800	0.96314400	2.19273800
H	-0.77652000	0.98489300	2.81538900
O	0.82917100	2.79794200	0.31131200
H	1.08826600	2.40557200	-0.54855600
O	1.41627400	1.01871900	-1.93958700
H	2.37902100	1.13363500	-1.86256800
O	-0.41731700	-2.17151600	-1.56328900
H	-0.76310800	-2.89702900	-1.01430200
O	-2.23492000	-1.52304300	1.04261700
H	-1.71701900	-2.25986800	1.41181400
H	-2.32178800	-0.89007000	1.78394300
H	-1.76595700	1.89664300	2.06610600
H	-0.08322700	3.09713500	0.15807300
H	1.14317300	1.65141100	-2.62627400
H	-1.10793900	-2.02804800	-2.23443000
O	0.89003500	-0.75969000	0.94118400
O	-1.70274500	0.75888500	-1.15112600
N	3.48820200	-0.43488500	0.50482800
O	4.26948600	-1.14848800	1.07562600
H	3.86606900	0.29925200	-0.12806100
H	2.41673300	-0.55437800	0.65230000

INT2

Atom	X	Y	Z (Angstrom)
Np	-0.41255600	0.01301600	-0.12633100
O	-1.68955600	0.81143200	1.99720100
H	-1.04820900	0.83189700	2.72992900
O	0.51699600	2.97668600	0.53115100
H	0.88811300	2.62111200	-0.30160700
O	1.31831700	1.32424900	-1.66109000
H	2.16288900	0.87332300	-1.83340500
O	-0.38819200	-2.17787700	-1.48649000
H	-0.13393000	-2.87298000	-0.85365900
O	-2.24419500	-1.80196000	0.85727700
H	-1.63895000	-2.43092700	1.28771100
H	-2.48179700	-1.18031500	1.57095100
H	-1.92858000	1.74475300	1.85589900
H	-0.38561700	3.23426000	0.28005100
H	0.91455600	1.45317700	-2.53741000
H	-1.32335400	-2.36500900	-1.68365600
O	0.91697100	-0.89052400	1.10304600
O	-1.68448200	0.76413800	-1.16134600
N	3.70710300	-0.43710000	0.37876300
O	4.69804800	-0.95385300	0.83537400
H	3.97556000	0.23704600	-0.38624500
H	1.86609400	-0.71544300	0.84790300

IC^{M}1

Atom	X	Y	Z (Angstrom)
Np	0.61677600	-0.26660200	0.05137200
O	0.60856700	-2.45646000	-1.25837700
H	0.44772600	-2.27738500	-2.20226300
O	2.38390400	0.77060300	-1.41372000
H	2.22970800	1.72654900	-1.13737700
O	1.73782900	3.17468400	-0.44041100
H	1.02044400	3.46716500	-1.02937100
O	0.38613200	1.66162900	1.63212600
H	-0.54481400	1.90681600	1.78683400
O	-1.17840700	-1.28807400	1.53214200
H	-1.99137900	-0.79650300	1.24254400
H	-1.30897800	-2.20375400	1.22501800
H	1.50191900	-2.84307800	-1.22230000
H	3.23389500	0.52453800	-1.00621700
H	1.26720200	2.80285500	0.33609000
H	0.77289100	1.50326400	2.51253200
O	-0.62427500	0.45658700	-0.96814300
O	1.86784000	-0.96727300	1.05851800
N	-4.02664700	-0.19860500	-0.41502600
O	-3.09044400	0.44174900	0.51509100
C	-4.99174200	0.82434300	-0.82258700
H	-5.77869000	0.32312100	-1.39570700
H	-4.49801900	1.54968900	-1.47547300
H	-5.44650600	1.35341700	0.02503900
H	-4.51044600	-0.83962300	0.21425300
H	-2.34727200	0.69349600	-0.06830100

TS^M1

Atom	X	Y	Z (Angstrom)
Np	0.62580700	-0.26324600	0.04939100
O	0.64545900	-2.46018300	-1.28862600
H	0.47329300	-2.22706000	-2.21859700
O	2.23044700	0.98507700	-1.52588900
H	2.03623400	1.88543700	-1.13066900
O	1.48432700	3.24546800	-0.21827900
H	0.83552500	3.67400200	-0.80241100
O	-0.10357600	1.78218700	1.62180600
H	-1.07032800	1.88639100	1.57405200
O	-0.97146500	-1.49918800	1.66634900
H	-1.84039100	-1.09201600	1.47154500
H	-1.04390200	-2.40902300	1.32543100
H	1.55788500	-2.80021300	-1.28513400
H	3.12880200	0.77303100	-1.21739500
H	0.93327200	2.83220400	0.48387800
H	0.09846900	1.66365700	2.56651200
O	-0.79133300	0.30471200	-0.92612600
O	2.04306300	-0.83652000	0.97306700
N	-4.05183400	-0.16735500	-0.14697200
O	-3.00163000	0.30450100	0.61471300
C	-4.43334600	0.68895800	-1.25732500
H	-5.28667300	0.22399600	-1.75410900
H	-3.59859100	0.76744100	-1.95828300
H	-4.70908900	1.69187700	-0.90384900
H	-4.80217200	-0.39263900	0.50520600
H	-2.23184600	0.43410300	-0.01291700

INT^M1

Atom	X	Y	Z (Angstrom)
Np	0.65469300	-0.26831100	0.06514600
O	0.72190700	-2.48240400	-1.25241700
H	0.56225700	-2.24219900	-2.18285100
O	2.27889100	0.96689800	-1.49476000
H	2.08786800	1.87217100	-1.10909900
O	1.54011100	3.25635500	-0.23172300
H	0.93238700	3.70629300	-0.84326600
O	-0.14507400	1.79182800	1.50627300
H	-1.11365200	1.84229500	1.40936200
O	-1.07013100	-1.42919600	1.59646400
H	-1.88804900	-0.95172700	1.31817100
H	-1.16292000	-2.31865600	1.20982800
H	1.62922900	-2.83597000	-1.24276600
H	3.16931600	0.74679000	-1.16861600
H	0.94368000	2.85299100	0.43763800
H	0.01378800	1.69035100	2.46151500
O	-0.85617000	0.18461500	-1.21731400
O	2.02828500	-0.71610300	1.16021000
N	-4.17618900	-0.00280000	0.06021800
O	-2.98155600	0.24073400	0.48031100
C	-4.67200100	0.63915500	-1.14223200
H	-5.62527500	0.18127700	-1.41097300
H	-3.94447000	0.49732000	-1.94524500
H	-4.81513500	1.71248700	-0.96742600
H	-4.82701300	-0.40070900	0.73930000
H	-1.71323500	0.28302300	-0.70860100

IC^M2

Atom	X	Y	Z (Angstrom)
Np	0.68868700	-0.05144900	-0.06069000
O	0.12840900	2.83643600	1.30574400
H	-0.57431400	2.18224400	1.46587500
O	0.14066900	-0.33879200	2.57371400
H	0.38549600	-1.28166100	2.47748900
O	1.06111600	-2.52268300	0.96429900
H	0.59892000	-3.17781100	0.41303300
O	1.08070700	-1.03560100	-2.51050000
H	0.34056600	-0.70636200	-3.04966100
O	0.36520700	2.33896000	-1.40084700
H	-0.54385800	2.23227400	-1.72899300
H	0.24820700	2.70609500	-0.48771200
H	0.92859600	2.37913400	1.61892900
H	0.90869500	0.05829500	3.02092800
H	2.00641300	-2.71411200	0.83671400
H	1.85467200	-0.54891400	-2.84456900
O	-1.17397800	-0.28117800	-0.30766500
O	2.48473800	0.15872000	0.17271000
N	-3.69087100	-0.11045500	-0.11103600
O	-4.16092600	0.98521900	-0.00874700
C	-4.52849000	-1.28991500	-0.15459700
H	-4.27814900	-1.81723800	-1.08434700
H	-5.57684400	-1.00482800	-0.09308100
H	-4.20743600	-1.93139800	0.67657100
H	-2.53940700	-0.20697000	-0.18183100

TS^{M}2

Atom	X	Y	Z (Angstrom)
Np	0.68831000	-0.05138700	-0.06062300
O	0.12800900	2.83696700	1.30497200
H	-0.57502900	2.18320600	1.46547800
O	0.13972300	-0.33841400	2.57373500
H	0.38524300	-1.28114600	2.47795300
O	1.06083500	-2.52236700	0.96452600
H	0.59903900	-3.17780600	0.41329200
O	1.08042400	-1.03550500	-2.51017200
H	0.34034100	-0.70682300	-3.04975100
O	0.36461600	2.33778300	-1.40104500
H	-0.54437800	2.23105600	-1.72940100
H	0.24752200	2.70580800	-0.48825800
H	0.92794600	2.37956400	1.61864500
H	0.90723400	0.05945500	3.02115000
H	2.00624100	-2.71373600	0.83764800
H	1.85440500	-0.54891900	-2.84435600
O	-1.17591300	-0.28200400	-0.30783600
O	2.48410700	0.15877300	0.17244800
N	-3.68701800	-0.11072400	-0.11089000
O	-4.15812000	0.98476900	-0.00862400
C	-4.52600500	-1.28948200	-0.15478300
H	-4.27578300	-1.81727100	-1.08425400
H	-5.57428000	-1.00375900	-0.09393500
H	-4.20625900	-1.93120300	0.67666000
H	-2.52942300	-0.20751200	-0.18203000

INTᴹ2

Atom	X	Y	Z (Angstrom)
Np	-0.77089900	-0.02802100	-0.03476800
O	1.66184500	-2.08447700	1.26031300
H	2.40468400	-1.76707100	0.70475500
O	0.73022600	0.71475800	2.05507900
H	0.43724800	1.63838000	1.88318300
O	-0.75256000	2.70943300	0.84985600
H	-0.60433700	3.34657500	0.13077900
O	-2.58558700	0.37584400	-1.82388400
H	-2.18454600	0.16361400	-2.68591400
O	-0.42447100	-2.56182200	-0.36515300
H	-0.07878300	-2.65268900	-1.27090200
H	0.39441900	-2.53415100	0.21258500
H	1.30397100	-1.25653200	1.63267400
H	0.21017800	0.44275400	2.83239700
H	-1.64243400	2.91113400	1.18561500
H	-3.28706800	-0.28955900	-1.70736200
O	0.64158000	0.28207600	-1.44807100
O	-2.07118900	-0.29884000	1.19036400
N	3.43809800	0.29546800	-0.58539200
O	3.85952900	-0.68073800	0.00286300
C	4.44580800	1.30574300	-0.89127900
H	4.39682100	1.49124700	-1.97051100
H	5.43956200	0.99399600	-0.56452000
H	4.11943400	2.22799400	-0.39389400
H	1.56792200	0.33767900	-1.08100900

IC^D1

Atom	X	Y	Z (Angstrom)
Np	-0.87013700	-0.03554400	0.09607000
O	-2.13427300	2.06458300	-0.69838300
H	-2.32572800	2.02388800	-1.65249300
O	-2.48759900	-1.59890600	-1.10859000
H	-2.00824400	-2.17847300	-1.72783000
O	0.09445700	-2.49118200	0.47524200
H	0.95303800	-2.46882500	0.01659700
O	1.18680100	0.03958800	1.51136100
H	2.01899300	-0.08229200	0.92300500
O	0.45394400	2.90524200	0.24745300
H	1.03791800	2.38852600	-0.33279200
H	-0.41931200	2.83048800	-0.18292200
H	-2.99899700	2.15159400	-0.25877600
H	-2.89240700	-2.20328900	-0.46070400
H	-0.48137100	-3.00622300	-0.11843000
H	1.15591400	-0.74172200	2.09216100
O	0.13229700	0.02161700	-1.34418700
O	-1.88559600	-0.09935800	1.51764200
N	3.33569300	-0.10093900	-0.08440800
O	2.99333500	0.77622200	-1.19464800
H	2.04959500	0.57565200	-1.35136200
C	3.70535500	-1.40312700	-0.65313400
H	3.97680400	-2.07373900	0.16756000
H	4.55077000	-1.31216200	-1.34812400
C	4.46830200	0.54792700	0.57934900
H	4.78790700	-0.09011200	1.40760800
H	5.30945500	0.69313000	-0.11230300
H	2.84405600	-1.81977000	-1.18264900
H	4.14560500	1.51424900	0.97342400

TS^D1

Atom	X	Y	Z (Angstrom)
Np	-0.81880700	-0.03813400	0.11601100
O	-2.27250800	1.84213400	-0.89692100
H	-2.41079700	1.78025600	-1.85818800
O	-2.42560100	-1.62765600	-1.12794700
H	-1.91013200	-2.08767200	-1.81422900
O	0.16214700	-2.51403700	0.47524900
H	1.01177100	-2.50059100	0.00084800
O	1.24089600	-0.07136400	1.74513200
H	2.03692600	-0.22804100	1.18940800
O	0.08823600	2.99096900	0.27653300
H	0.71245100	2.51721200	-0.29856000
H	-0.76819600	2.86181900	-0.17828200
H	-3.16307200	1.86264800	-0.50478400
H	-2.69508600	-2.33108000	-0.51085200
H	-0.43029400	-3.01114200	-0.11726900
H	1.09703800	-0.91951500	2.20255900
O	0.20325500	0.04332800	-1.37628900
O	-1.87095200	-0.12695100	1.55483000
N	3.40004200	-0.02779700	-0.19685600
O	2.71859300	0.98798900	-0.83982700
H	1.84506100	0.60022700	-1.13298600
C	3.57103900	-1.22650300	-1.01385300
H	3.97802400	-2.01736100	-0.38160700
H	4.26201900	-1.01689700	-1.84240000
C	4.57072300	0.50500700	0.48201300
H	5.01779700	-0.30285200	1.06416900
H	5.30076900	0.87955300	-0.24902800
H	2.60257800	-1.52798500	-1.41737100
H	4.25876200	1.31615100	1.14253300

INT^D1

Atom	X	Y	Z (Angstrom)
Np	-0.80911500	-0.04684300	0.13436800
O	-2.28754600	1.83660000	-1.03893700
H	-2.43685800	1.59381500	-1.96943400
O	-2.41357000	-1.66393100	-1.08251700
H	-1.87811900	-2.12452700	-1.75352000
O	0.19822400	-2.49971400	0.51781400
H	1.03342100	-2.47297800	0.01759600
O	1.00825300	0.34067100	1.92994600
H	1.86322300	0.05108300	1.56692800
O	0.14193400	2.98449500	0.03952000
H	0.77083800	2.40734800	-0.42634800
H	-0.69941400	2.82134700	-0.43040200
H	-3.17440900	1.89093700	-0.64229400
H	-2.68075700	-2.36391900	-0.46025900
H	-0.40318400	-3.00299500	-0.06001500
H	0.81659600	-0.29721000	2.64049100
O	0.26138000	-0.03201300	-1.57863200
O	-1.91137900	-0.16568000	1.56358500
N	3.49940000	-0.00693500	-0.31235100
O	2.68186100	0.86722900	-0.81148000
H	1.20734200	0.25704400	-1.37772900
C	3.67997200	-1.27318500	-1.01552600
H	4.06804500	-2.01928200	-0.31910500
H	4.39282300	-1.14464600	-1.84065800
C	4.54154400	0.48139800	0.58605300
H	4.87981100	-0.33913100	1.22261400
H	5.39236700	0.86304300	0.00663300
H	2.71535900	-1.59064900	-1.41530700
H	4.12243900	1.28513300	1.19349700

IC^D2

Atom	X	Y	Z (Angstrom)
Np	-0.74938800	-0.07317500	-0.14626100
O	-2.52057200	2.52701100	0.82144200
H	-2.74739800	1.61696600	1.09699500
O	-2.58362100	-0.42595200	1.66766900
H	-3.16238900	-1.15354000	1.38016000
O	-0.61611300	-2.74917400	0.51120100
H	-1.32324100	-3.12081300	-0.04474900
O	1.04393200	-1.54358800	-1.57761300
H	0.92309600	-2.25290700	-0.91777200
O	-0.43878600	2.41951400	-1.09673300
H	-0.84164100	2.34764400	-1.97952300
H	-1.19850700	2.65554200	-0.50797500
H	-2.02562900	2.87483600	1.58318500
H	-2.16968900	-0.74566400	2.48820600
H	-1.03299300	-2.65424100	1.38645800
H	1.90639300	-1.15195200	-1.35224700
O	-2.02355300	-0.35069200	-1.43826100
O	0.52328100	0.20195500	1.16389500
N	4.04110900	0.21733600	0.16718700
O	3.67545500	0.14842300	-0.97200700
C	3.54018400	-0.73297400	1.15595800
H	2.53857000	-0.35304100	1.43314100
H	4.20814900	-0.74703500	2.01491100
C	4.95043600	1.28577000	0.58492200
H	4.49576500	1.77878600	1.45036300
H	5.87727500	0.79972000	0.91212800
H	3.43047100	-1.70100400	0.66558300
H	5.10314000	1.95386200	-0.25895200

TSᴰ2

Atom	X	Y	Z (Angstrom)
Np	-0.67811500	-0.08638300	-0.14006800
O	-2.42423600	2.66623000	0.62487100
H	-2.64263200	1.75138900	0.88289300
O	-2.51072100	-0.43907900	1.65832400
H	-3.03811100	-1.20602400	1.37303600
O	-0.62150600	-2.73085000	0.52048700
H	-1.31684100	-3.10314000	-0.05019000
O	1.10496300	-1.57875500	-1.55230700
H	0.98312000	-2.30275300	-0.90977300
O	-0.32199100	2.37518200	-1.14879200
H	-0.68961700	2.27144100	-2.04363100
H	-1.09990700	2.64992900	-0.59683300
H	-1.96744900	3.01912500	1.40815400
H	-2.08368300	-0.72828200	2.48411900
H	-1.05184500	-2.65086800	1.39076300
H	2.00007000	-1.23503300	-1.36559600
O	-1.94057400	-0.35723700	-1.42679400
O	0.61623800	0.20542900	1.23924200
N	3.73076000	0.17945300	0.22636900
O	3.61949800	-0.07216100	-0.97104400
C	3.12344500	-0.59469400	1.19712500
H	1.93737200	-0.16816400	1.22083200
H	3.53835600	-0.42459900	2.18821000
C	4.44139600	1.41518500	0.61672800
H	3.81606700	1.95492600	1.33109800
H	5.37476800	1.11671100	1.10237600
H	3.00247400	-1.62960700	0.87936900
H	4.62484800	1.98939500	-0.28806900

INT^D2

Atom	X	Y	Z (Angstrom)
Np	-0.71189300	-0.14779700	-0.19022300
O	-2.96292900	2.23354500	1.02306800
H	-2.92632600	1.27786100	1.24439900
O	-2.52235800	-0.54317000	1.61376000
H	-3.10595000	-1.28370700	1.37095700
O	-0.20503600	-2.52414900	0.75243400
H	-0.49758900	-3.12437400	0.04316400
O	1.36134800	-0.92557500	-1.50722100
H	1.59729400	-1.79460700	-1.13723200
O	-1.25467800	2.21954800	-1.09576600
H	-1.78099600	2.08122100	-1.90256800
H	-1.93224700	2.37829700	-0.37655500
H	-2.45025600	2.65375400	1.73532500
H	-2.12745600	-0.79170700	2.46879400
H	-0.88133600	-2.62898900	1.44664400
H	2.01271500	-0.29127200	-1.09391700
O	-1.82557800	-0.86947300	-1.40538900
O	0.56925300	0.66169600	1.13501500
N	4.01856200	0.30999200	0.28429400
O	2.91245000	0.85129900	-0.19837900
C	4.10624800	-0.91676800	0.66784300
H	1.48986500	0.72026500	0.72003500
H	5.05268300	-1.28456400	1.03982900
C	5.15645400	1.24352500	0.33143300
H	6.04009600	0.73839200	0.71910400
H	5.32785500	1.60377800	-0.68446900
H	3.22962500	-1.54905500	0.59861800
H	4.87210700	2.07955300	0.97271200