Supplementary Electronic Information for:

Reduction of Np(VI) with Hydrazinopropionitrile via Water-mediated Proton Transfer

Xiao-Bo Li, [†,‡] Qun-Yan Wu,[*,†] Cong-Zhi Wang, [†] Jian-Hui Lan, [†] Meng Zhang, [‡]

John K. Gibson, [&] Zhi-Fang Chai, [†] and Wei-Qun Shi[*,†]

[†]Laboratory of Nuclear Energy Chemistry, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China

[‡]Fundamental Science on Nuclear Safety and Simulation Technology Laboratory, College of Nuclear Science and Technology, Harbin Engineering University, Harbin, Heilongjiang, 150001, China

[&]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

Email: wuqy@ihep.ac.cn, shiwq@ihep.ac.cn

*To whom correspondence should be addressed

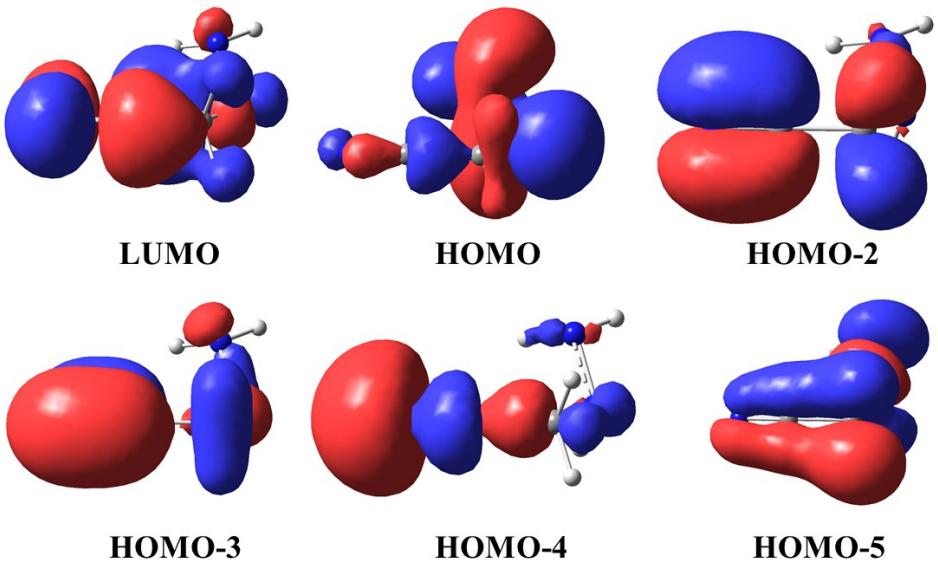

Fig. S1 Molecular orbitals of $NCCH_2N_2H_3$ at the B3LYP/6-31G(d) level of theory. The isosurface value of the MOs is set to be 0.03 au.

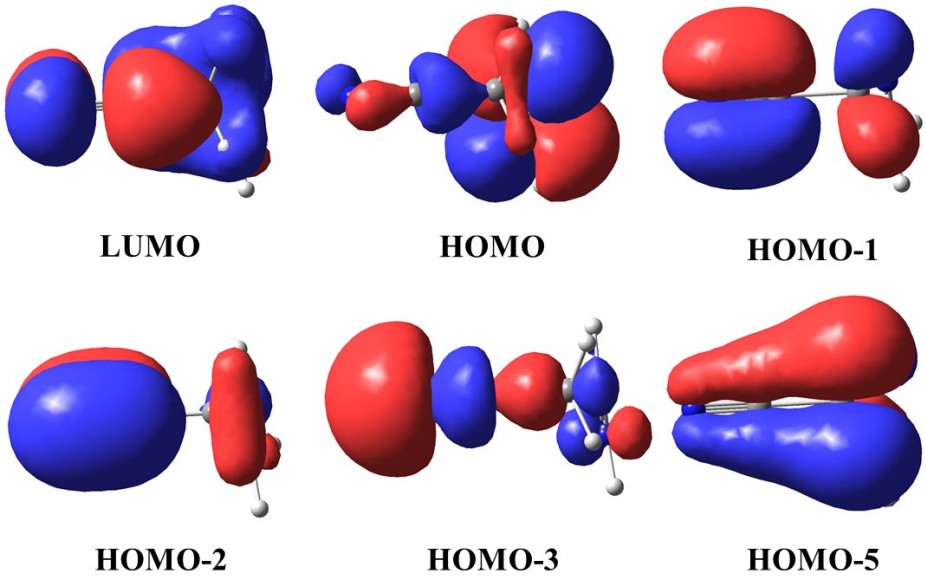

Fig. S2 Molecular orbitals of $NCCH_2N_2H_3^{+\bullet}$ at the B3LYP/6-31G(d) level of theory. The isosurface value of the MOs is set to be 0.03 au.

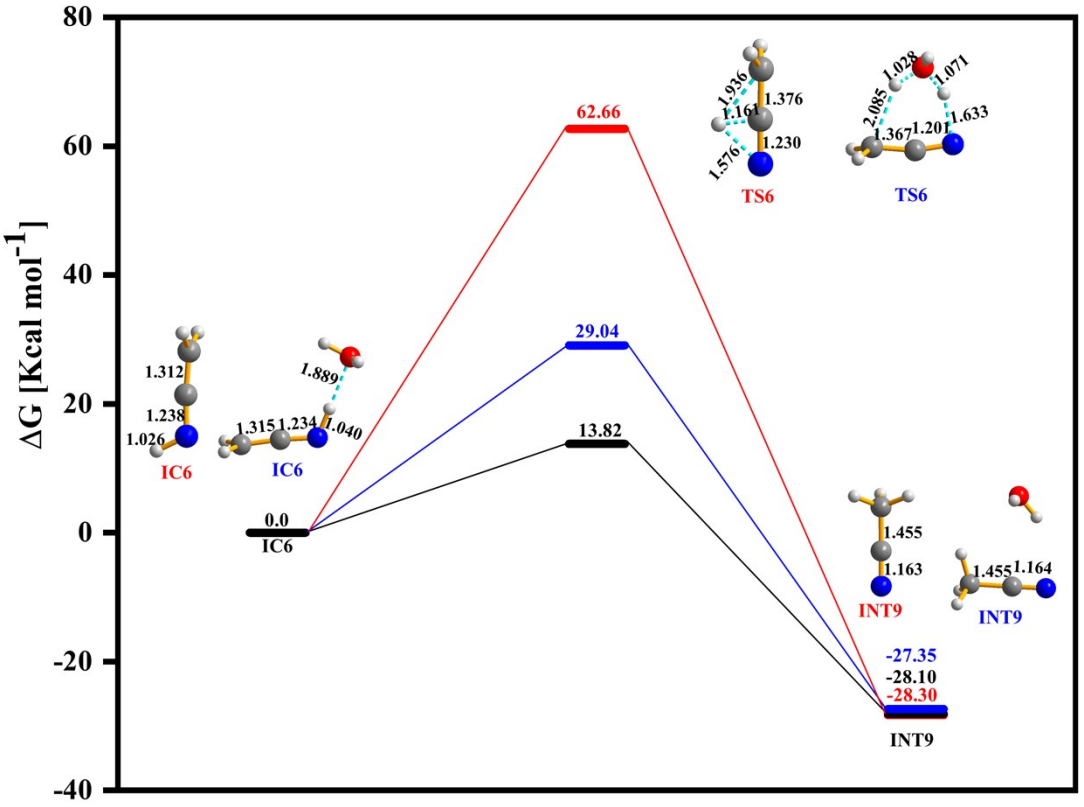

Fig. S3 Potential energy profiles for the isomerization between CH_2CNH and CH_3CN of the two, one, and without water-assisted proton transfer at the B3LYP/6-31G(d) level of theory.

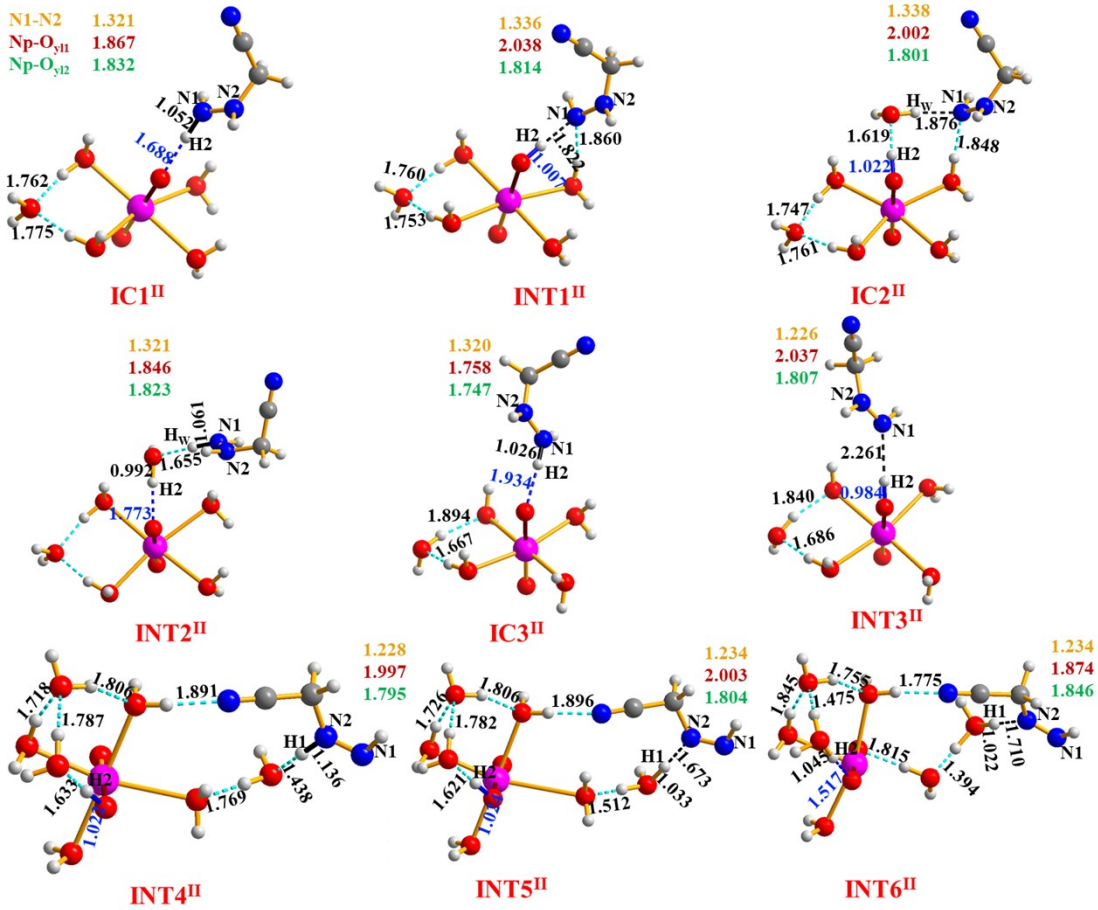

Fig. S4 Optimized structures and related bond distances (Å) of ICs and INTs for pathway II of the neptunyl species with hydrazinopropionitrile in the aqueous phase at the B3LYP/ECP60MWB/6-31G(d) level of theory.

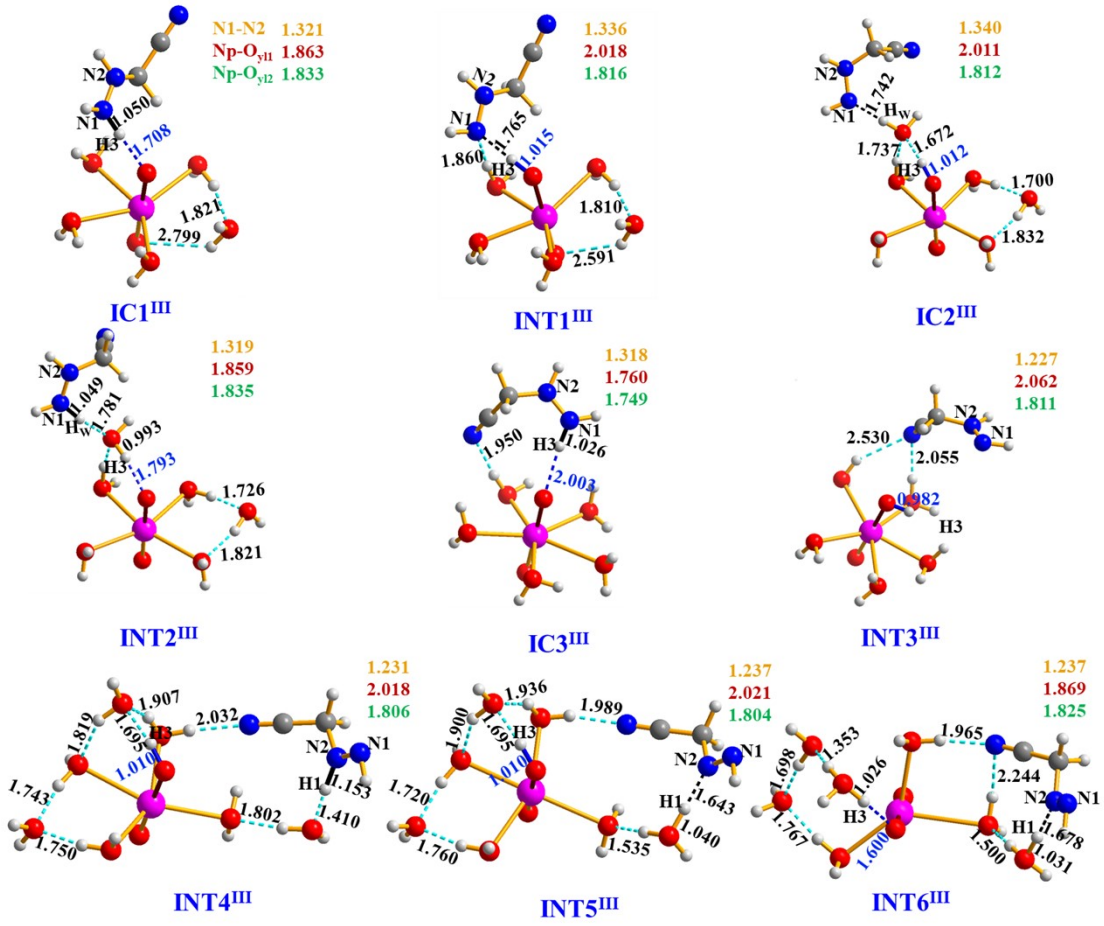

Fig. S5 Optimized structures and related bond distances (Å) of ICs and INTs for pathway III of the neptunyl species with hydrazinopropionitrile in the aqueous phase at the B3LYP/ECP60MWB/6-31G(d) level of theory.

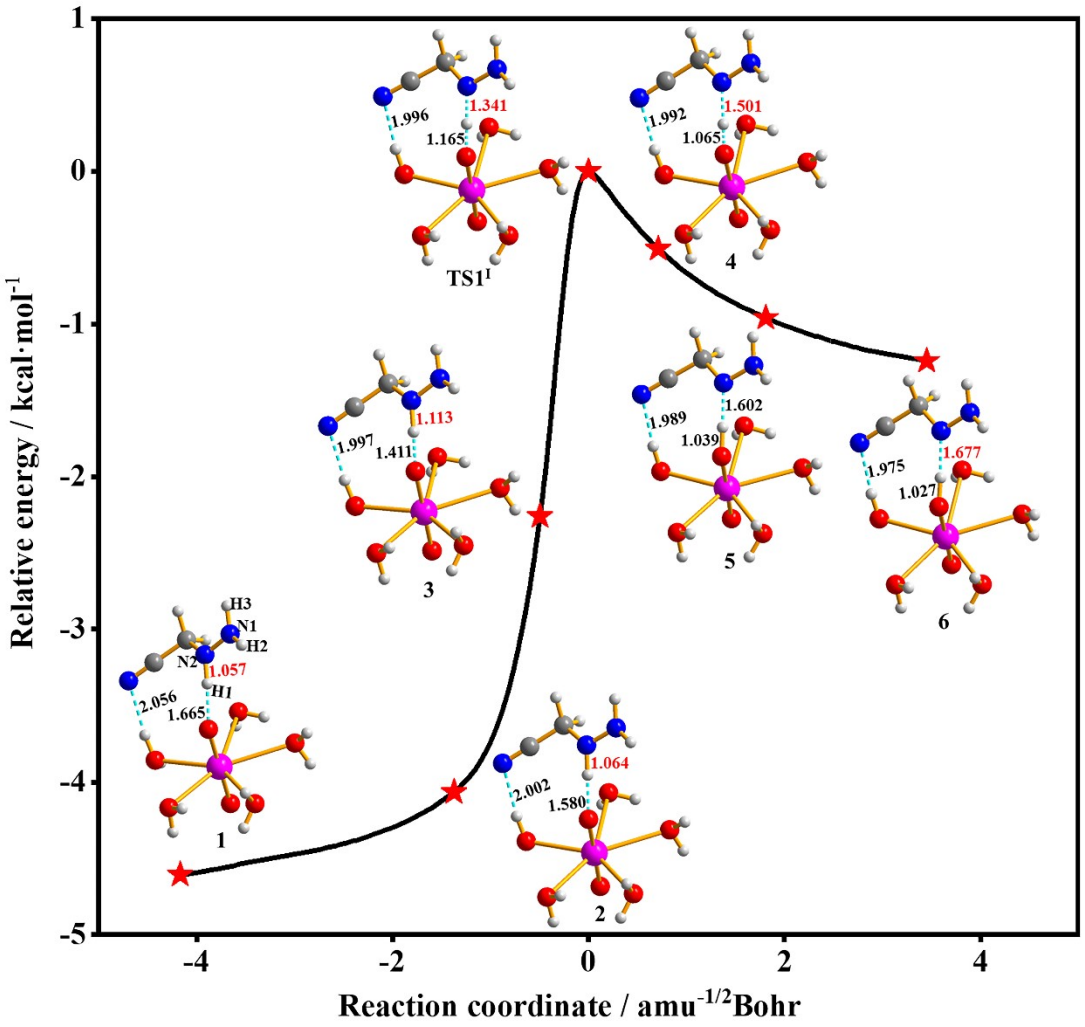

Fig. S6 IRC of TS1[I] and the structures of the corresponding IRC.

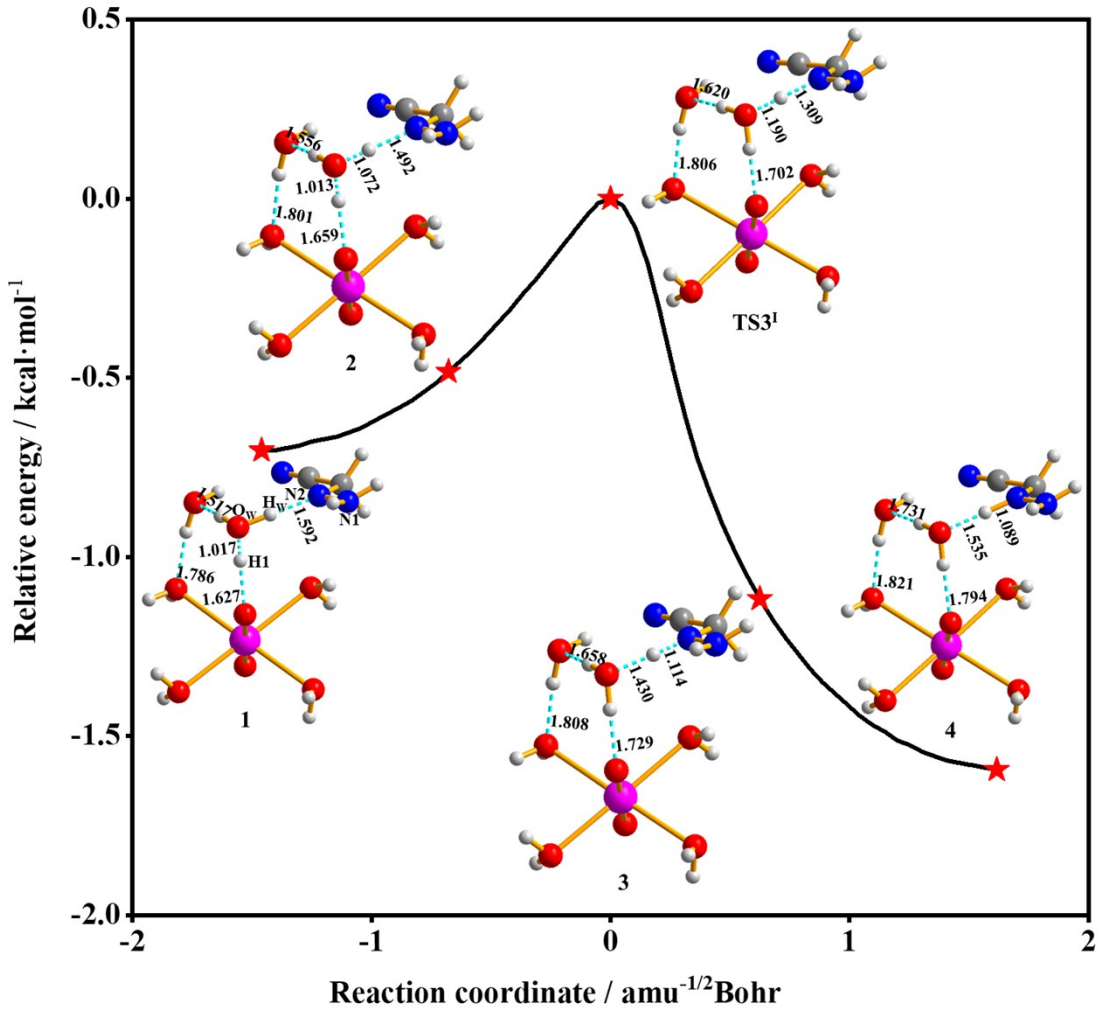

Fig. S7 IRC of $TS3^{I}$ and the structures of the corresponding IRC.

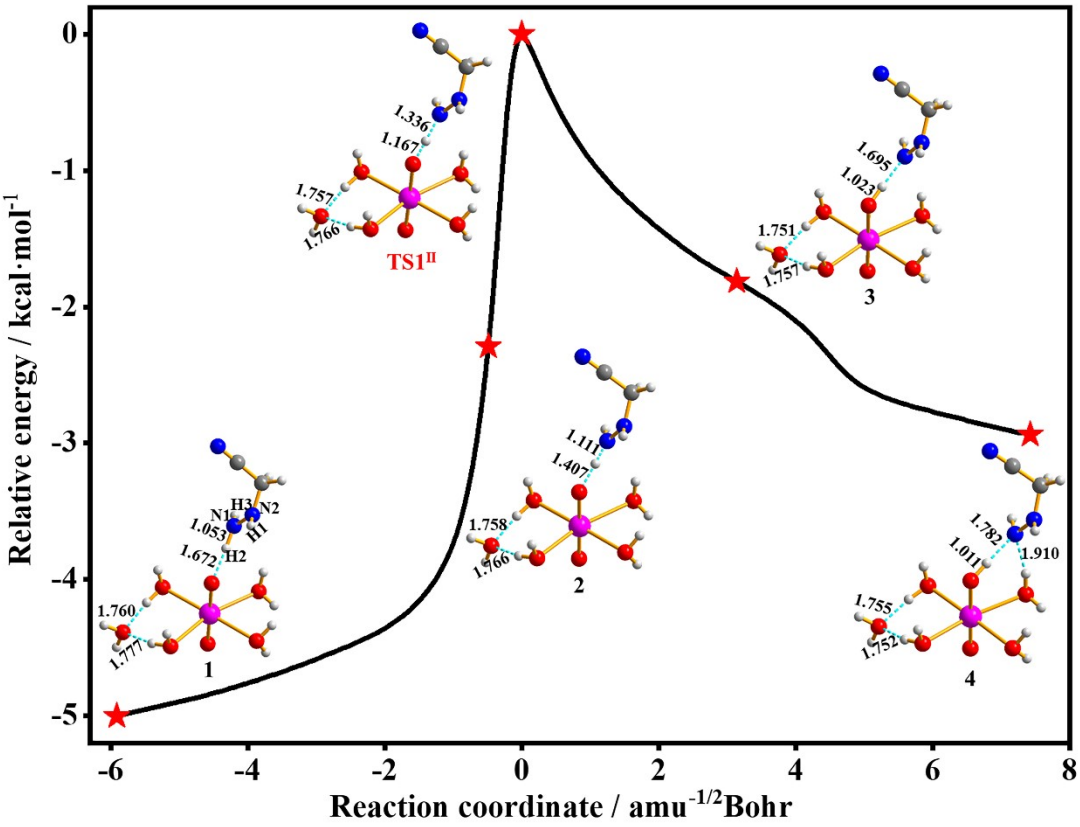

Fig. S8 IRC of $TS1^{II}$ and the structures of the corresponding IRC.

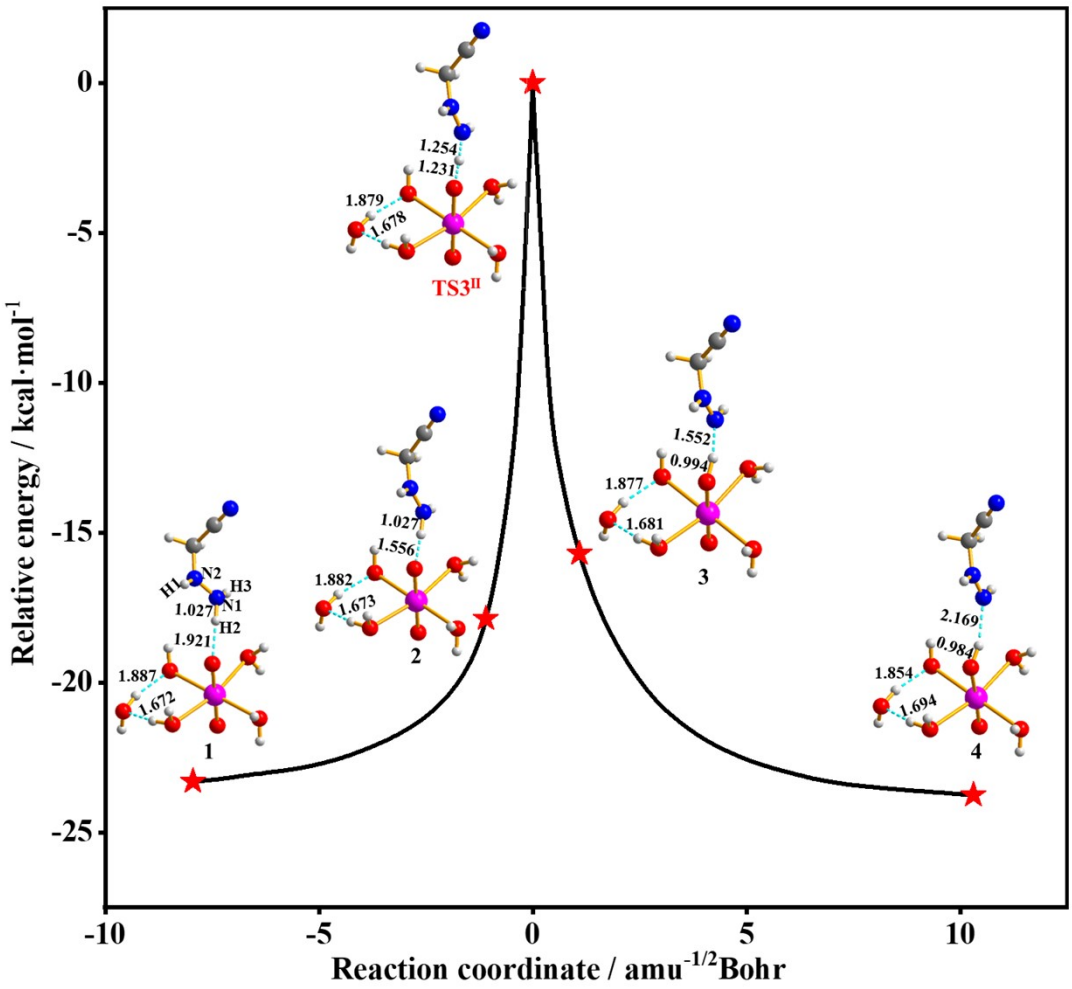

Fig. S9 IRC of $TS3^{II}$ and the structures of the corresponding IRC.

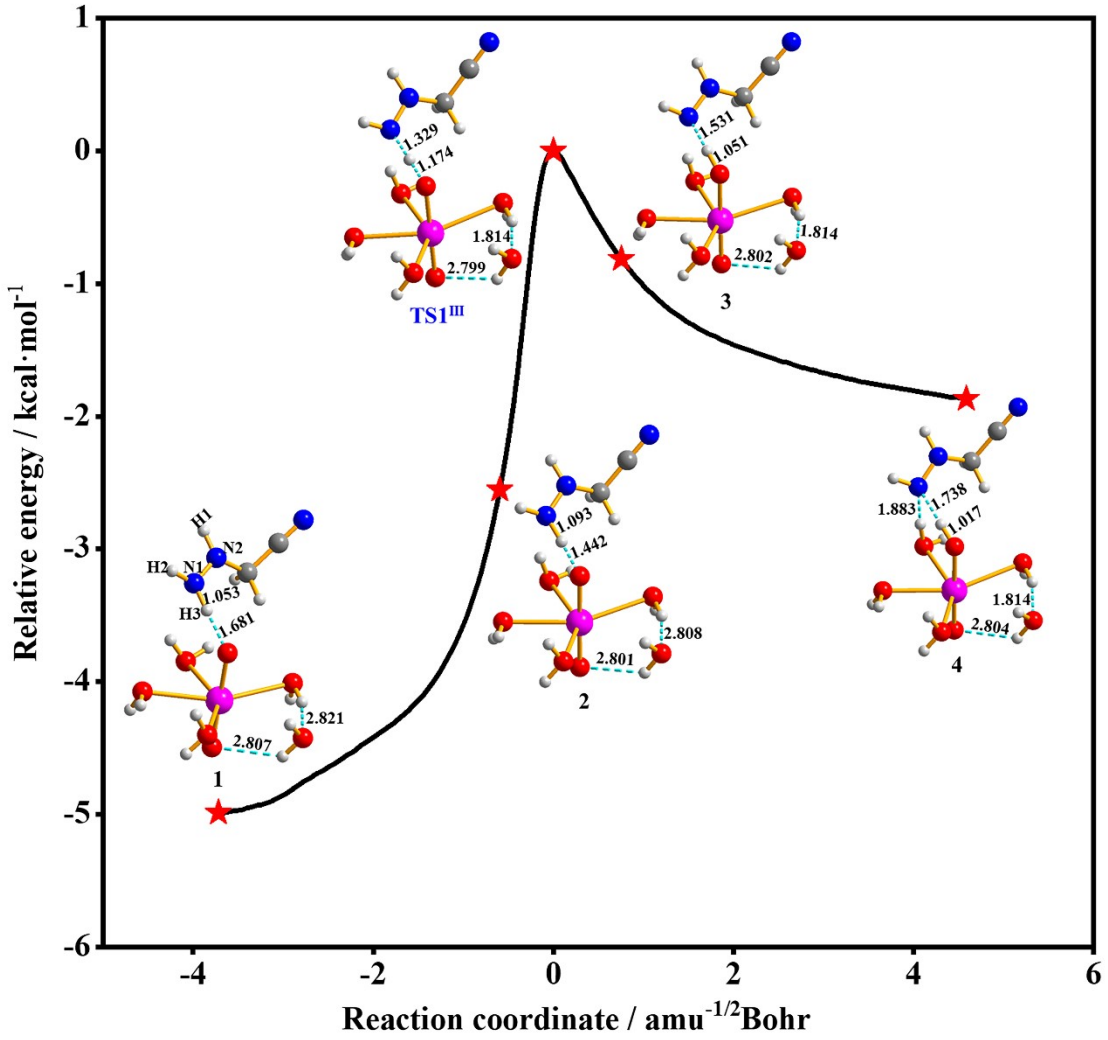

Fig. S10 IRC of TS1^{III} and the structures of the corresponding IRC.

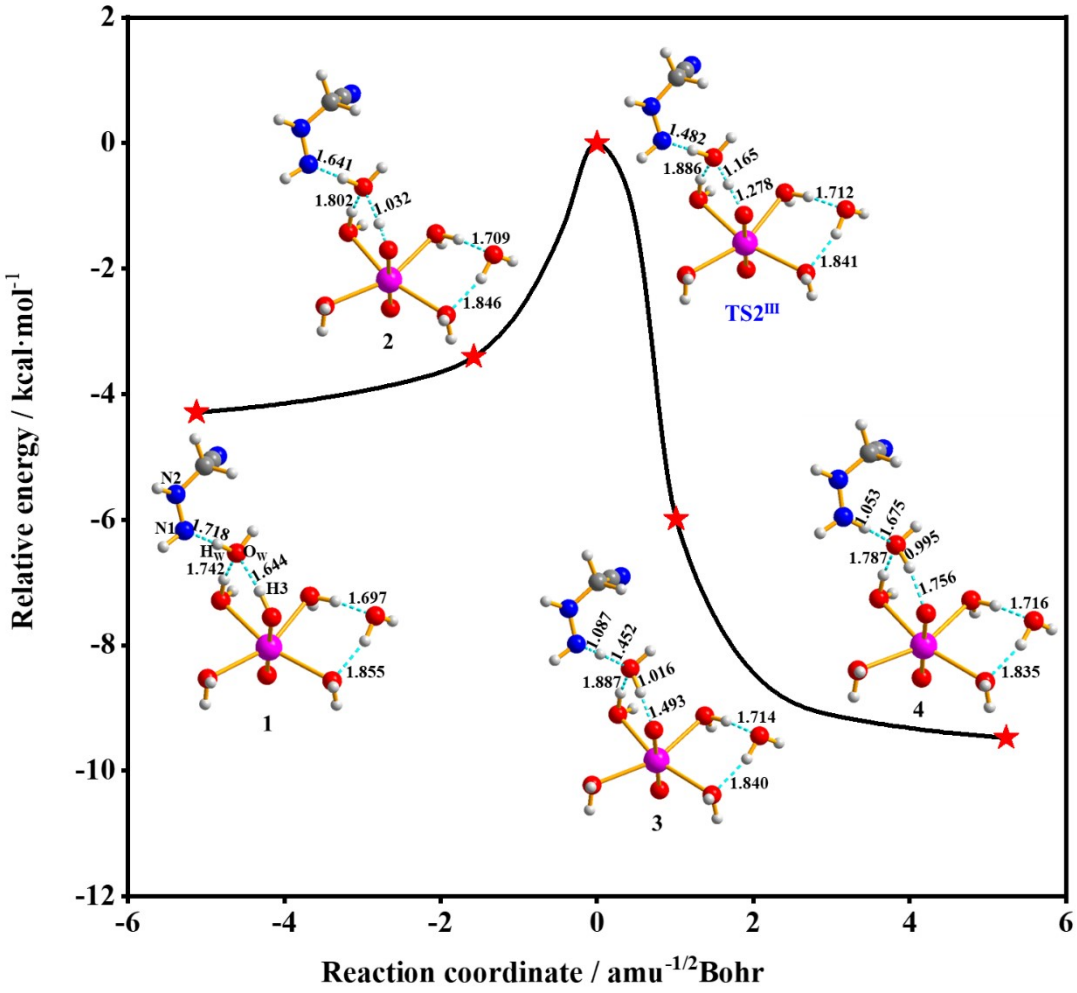

Fig. S11 IRC of TS2^{III} and the structures of the corresponding IRC.

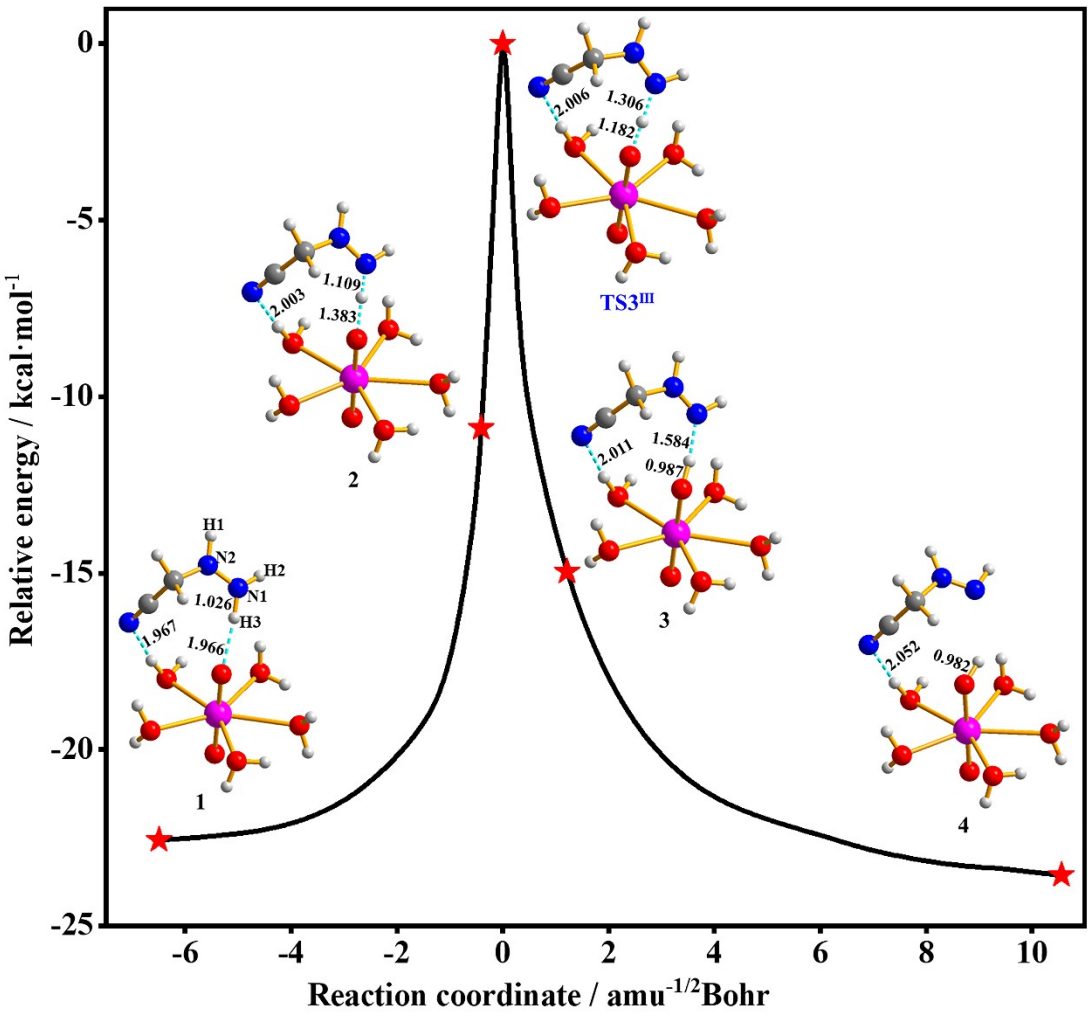

Fig. S12 IRC of TS3^{III} and the structures of the corresponding IRC.

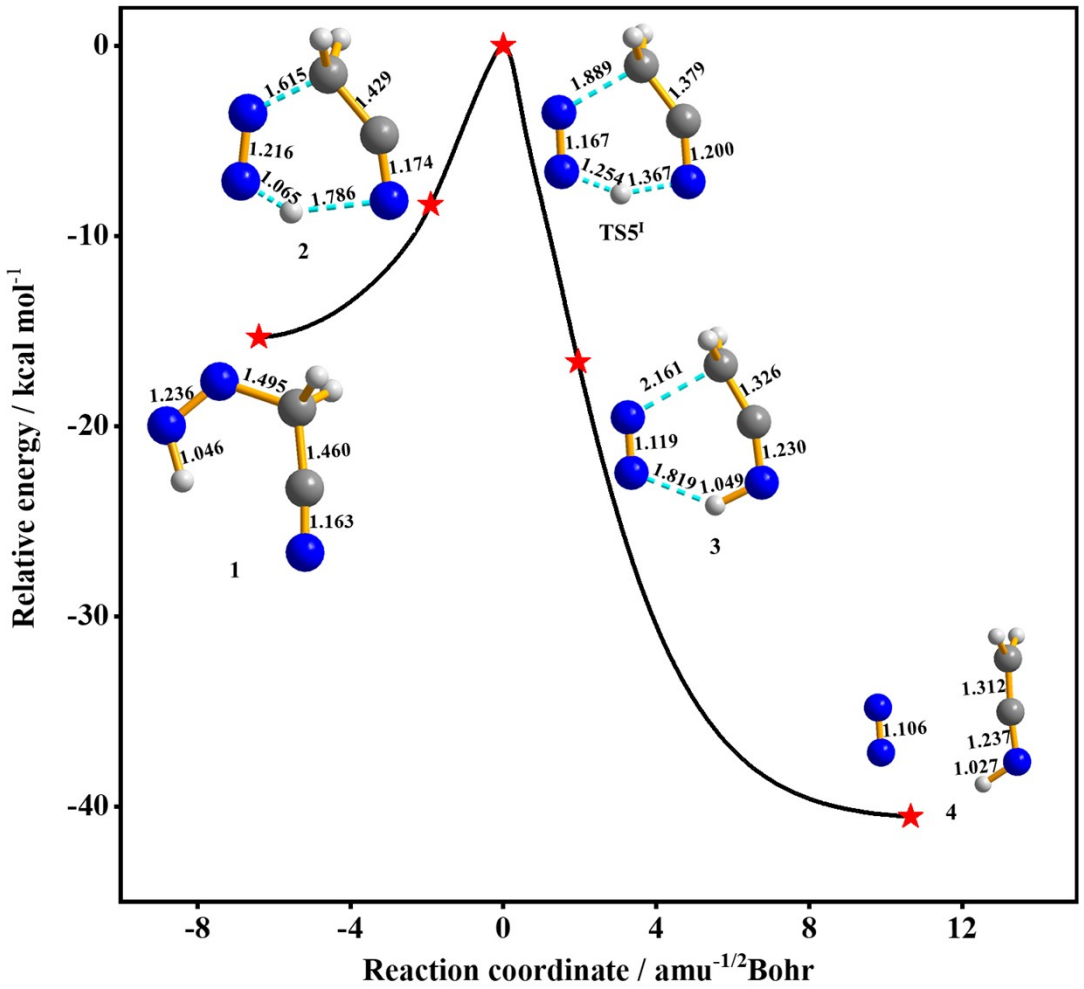

Fig. S13 IRC of TS5[I] and the structures of the corresponding IRC.

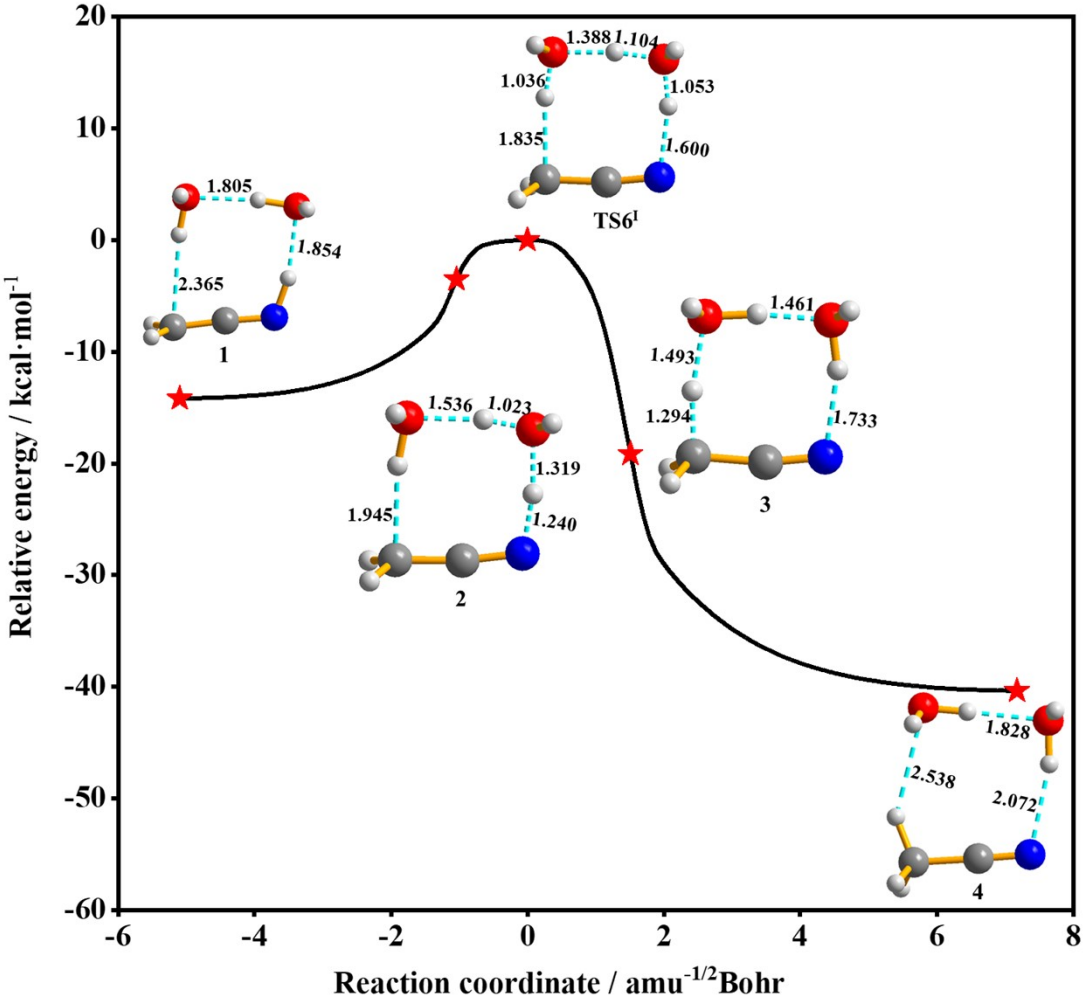

Fig. S14 IRC of TS6[I] and the structures of the corresponding IRC for double-water-assisted proton transfer.

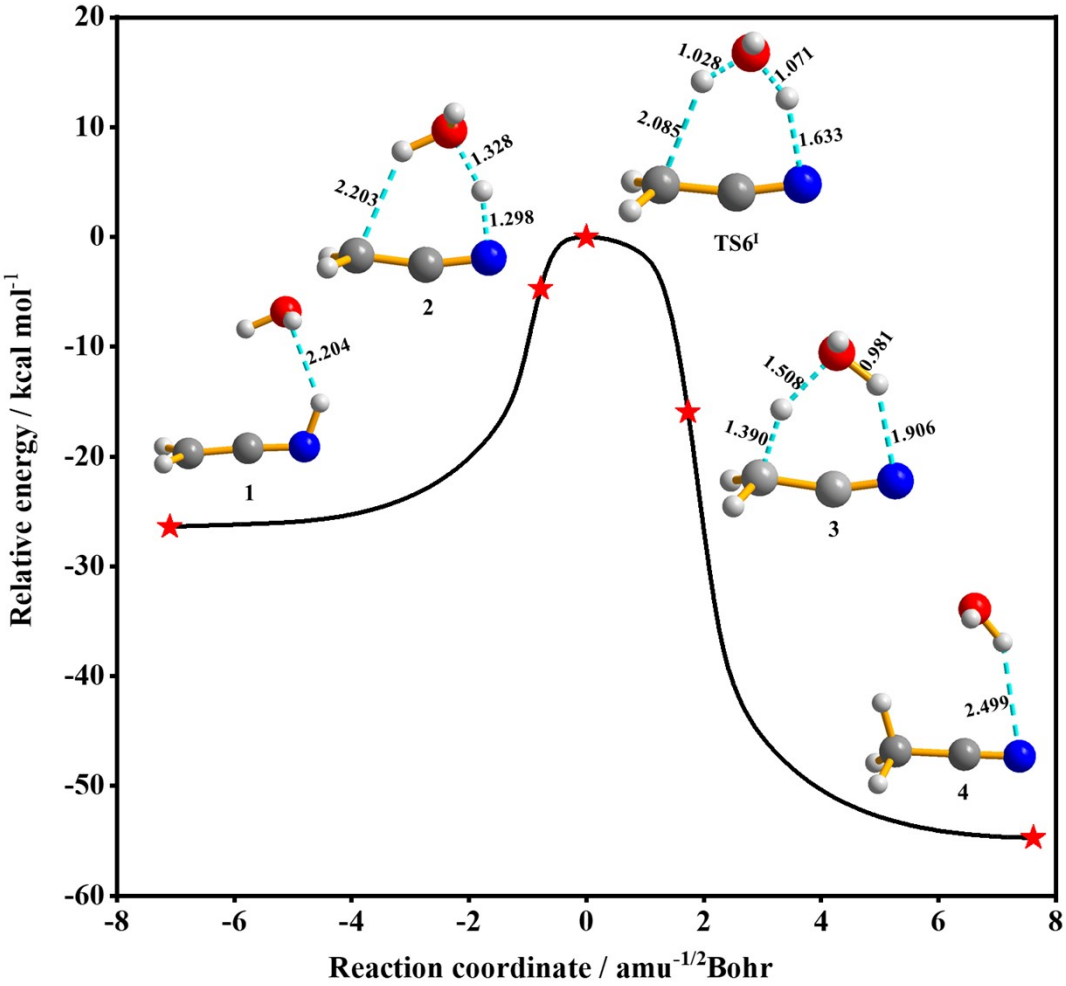

Fig. S15 IRC of TS6[I] and the structures of the corresponding IRC for a water-assisted proton transfer.

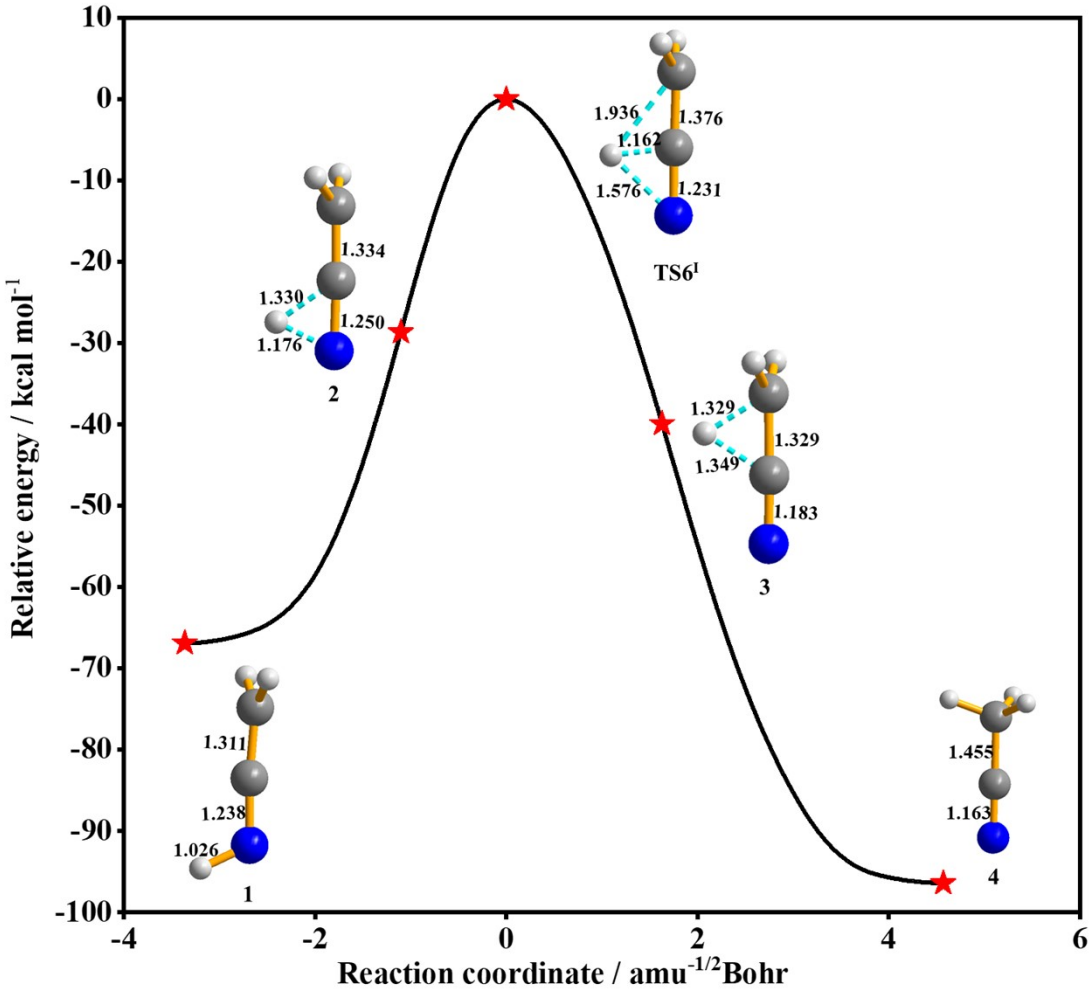

Fig. S16 IRC of TS6^{I} and the structures of the corresponding IRC for without water-assisted proton transfer.

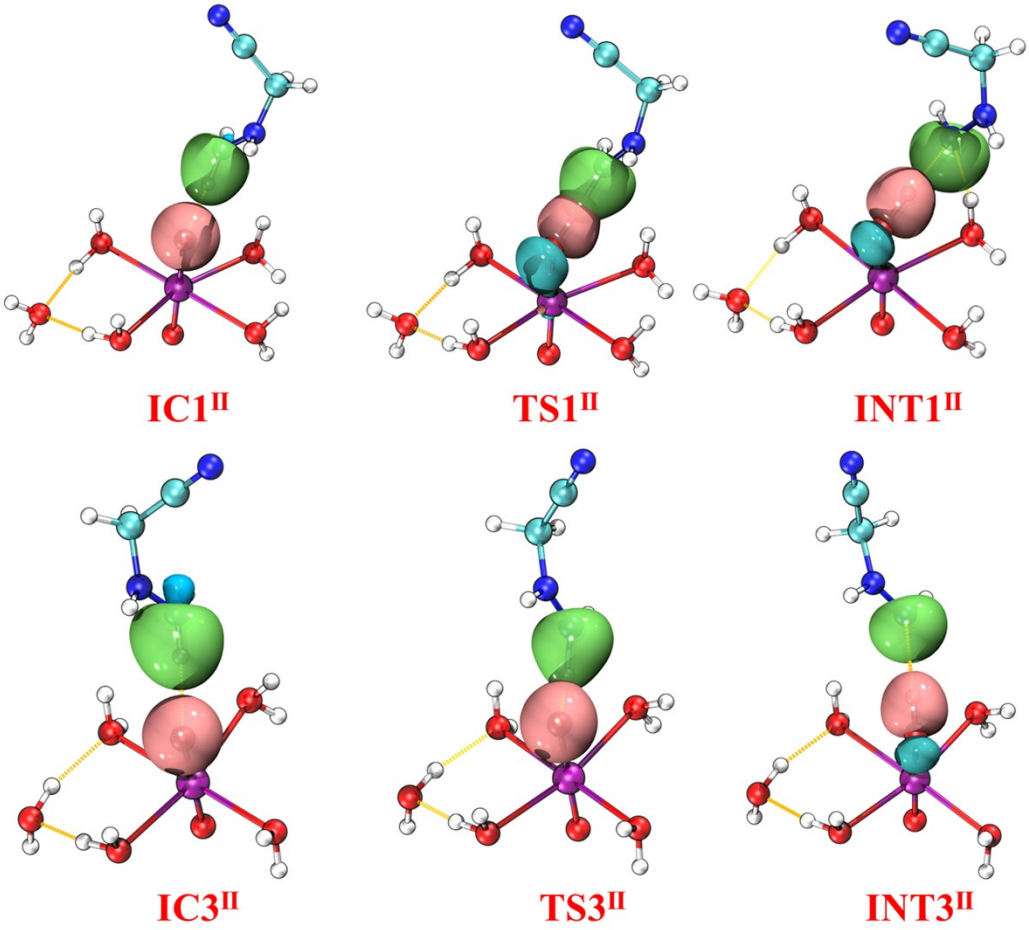

Fig. S17 Diagrams of LMOs (isovalue = 0.08) for the structures of pathway II. The yellow dashed lines indicate the hydrogen bond. The purple, red, blue, cyan, white balls represent Np, O, N, C, H atoms, respectively.

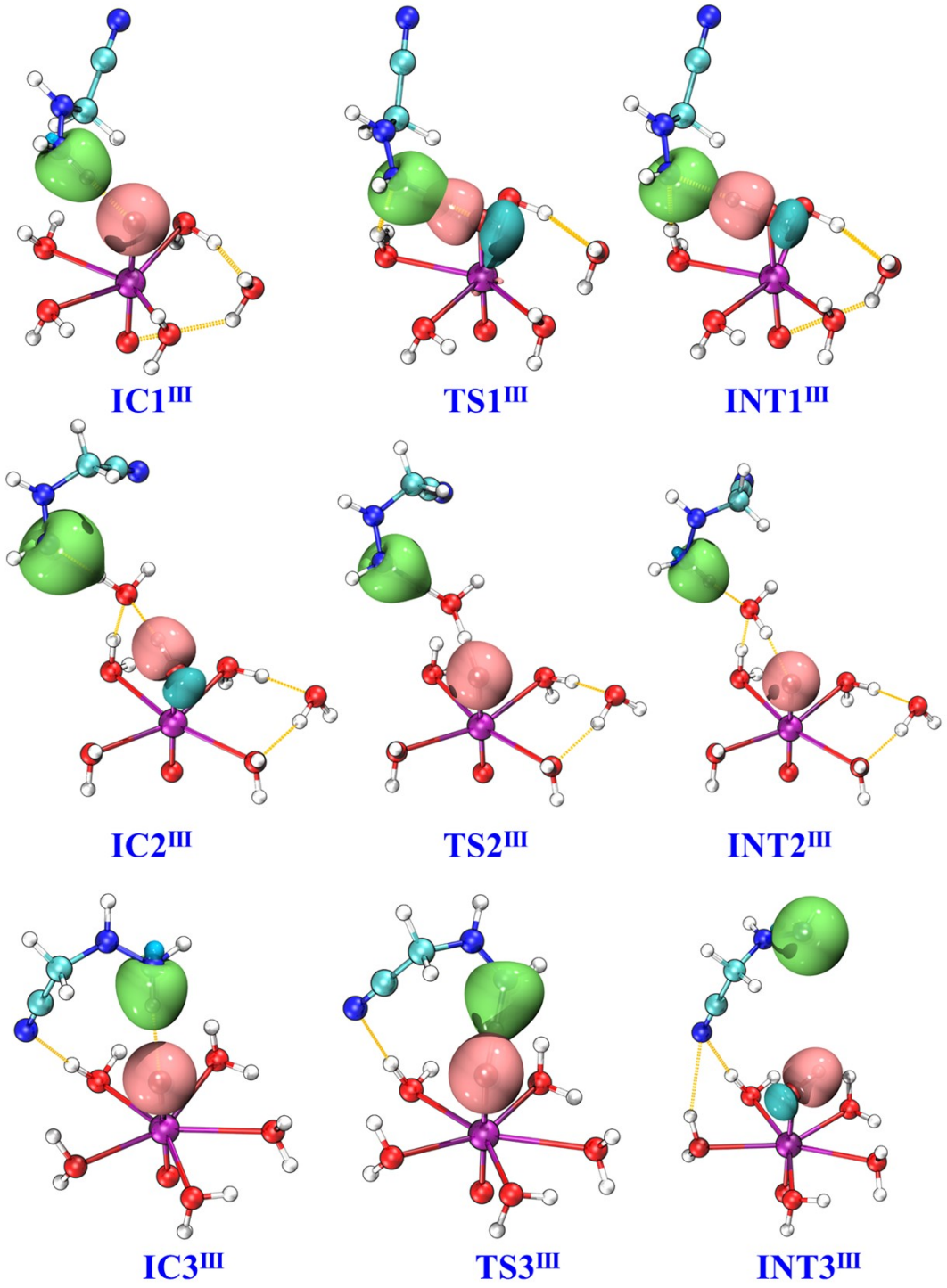

Fig. S18 Diagrams of LMOs (isovalue = 0.08) for the structures of pathway III. The yellow dashed lines indicate the hydrogen bond. The purple, red, blue, cyan, white balls represent Np, O, N, C, H atoms, respectively.

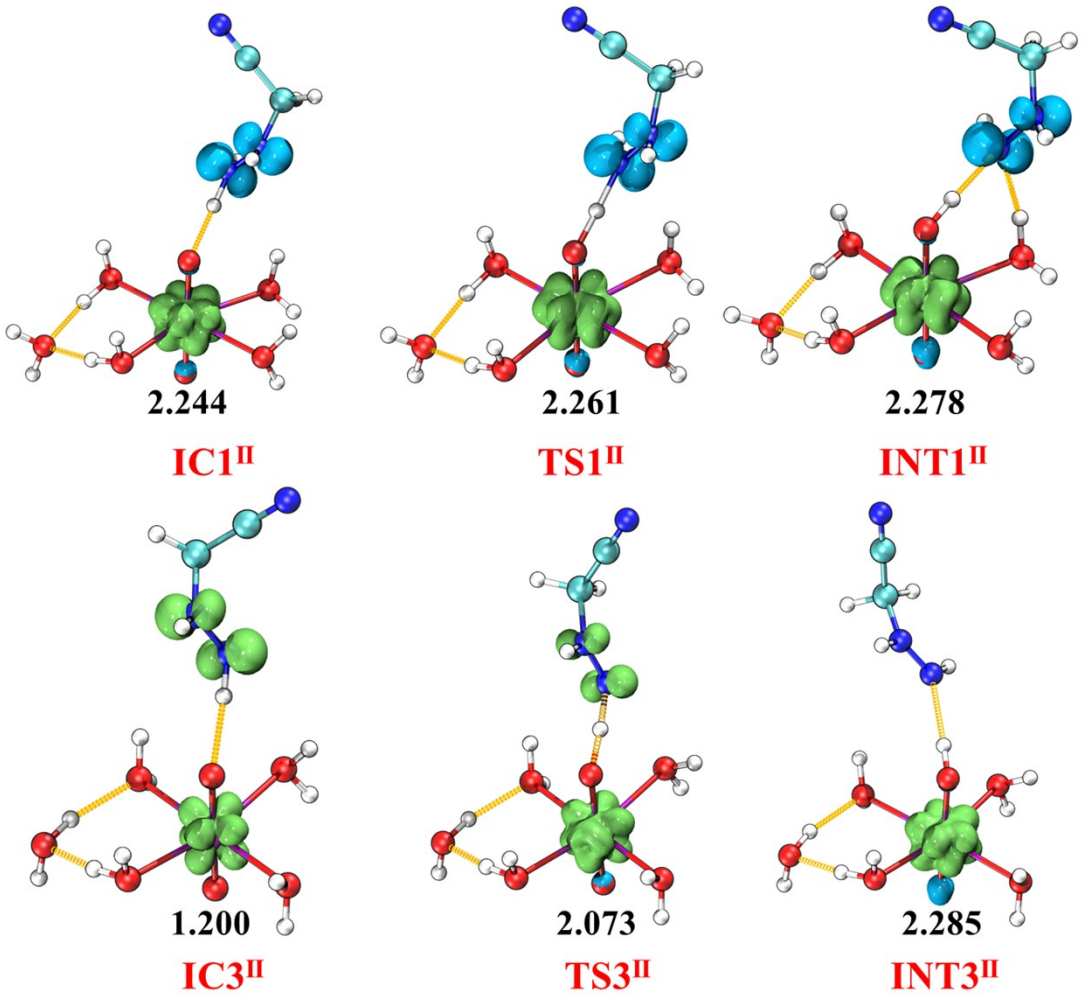

Fig. S19 Diagrams of spin density (isovalue = 0.02) and the value of the spin density on the Np atom for the structures of pathway II.

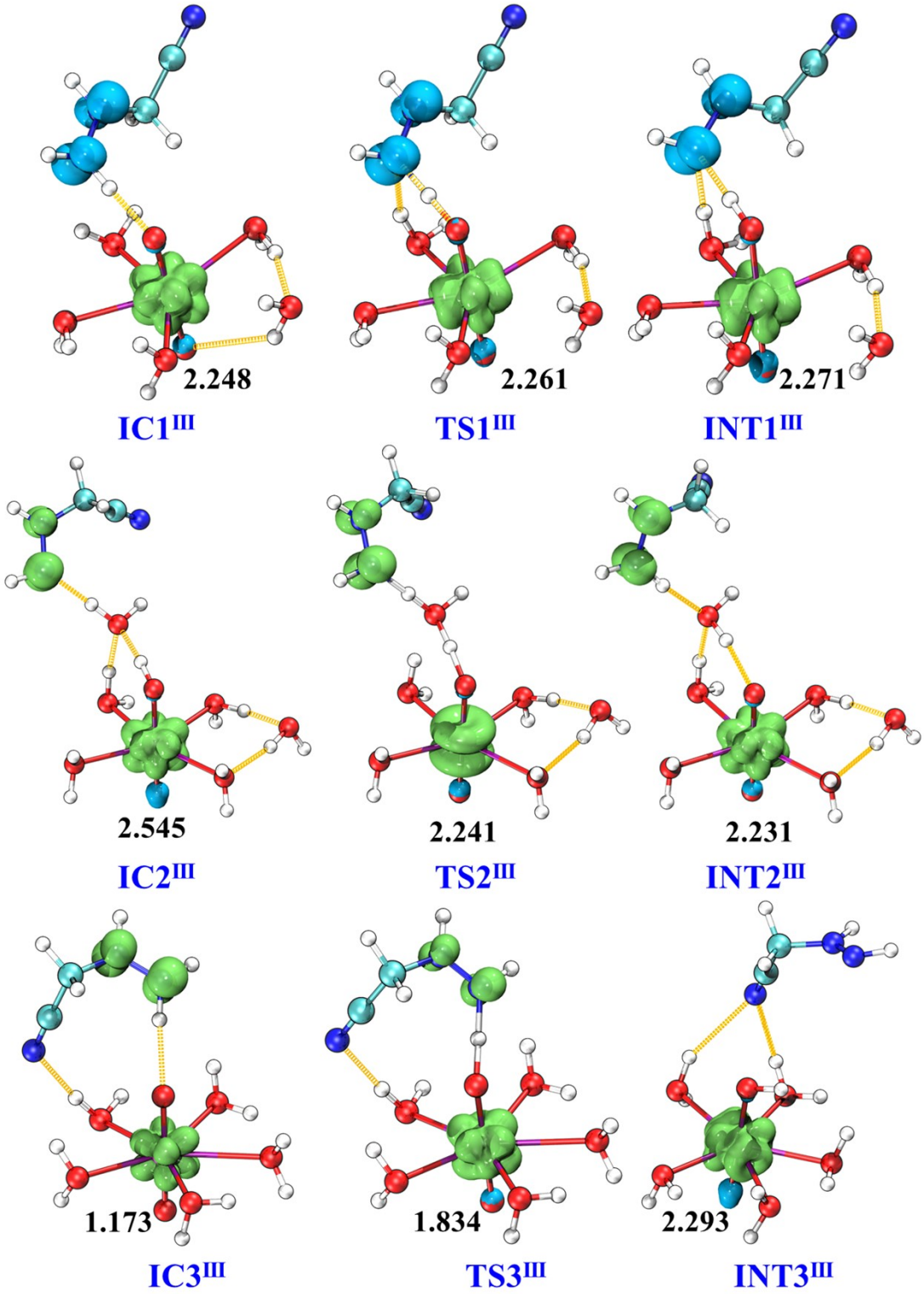

Fig. S20 Diagrams of spin density (isovalue = 0.02) and the value of the spin density on the Np atom for the structures of pathway III.

Table S1 Electronic energy (E) of the structures for the first stage of three pathways

Complexes	E (a.u.)
$IC1^{I}$	-1290.5068343
$TS1^{I}$	-1290.5046454
$INT1^{I}$	-1290.5066098
$IC1^{II}$	-1290.5162506
$TS1^{II}$	-1290.5038334
$INT1^{II}$	-1290.5088767
$IC1^{III}$	-1290.5101527
$TS1^{III}$	-1290.4974135
$INT1^{III}$	-1290.5007048

Table S2 Electron density [ρ(r), au], its Laplacian [$\nabla^2\rho$(r), au], total energy density [H(r), au], and MBOs of the O-H, N-H and O_{yl1}-H bonds of the structures for pathway I

$NCCH_2N_2H_3$	bond	ρ(r)	$\nabla^2\rho$(r)	H(r)	MBOs
$IC2^{I}$	O_w-H1	0.073	0.177	-0.012	0.308
	O_{yl1}-H1	0.260	-1.111	-0.344	0.421
$INT2^{I}$	O_w-H1	0.282	-1.376	-0.401	0.548
	O_{yl1}-H1	0.055	0.164	-0.003	0.159
$IC3^{I}$	O_w-H_w	0.263	-1.158	-0.352	0.514
	N2-H_w	0.065	0.139	-0.010	0.252
$TS3^{I}$	O_w-H_w	0.174	-0.366	-0.173	0.398
	N2-H_w	0.141	-0.153	-0.102	0.326
$INT3^{I}$	O_w-H_w	0.070	0.180	-0.009	0.310
	N2-H_w	0.261	-1.183	-0.340	0.493
$IC4^{I}$	N2-H1	0.318	-1.637	-0.443	0.690
	O_{yl1}-H1	0.022	0.075	0.000	0.064
$TS4^{I}$	N2-H1	0.298	-1.498	-0.409	0.535
	O_{yl1}-H1	0.043	0.135	-0.001	0.184
$INT4^{I}$	N2-H1	0.015	0.047	0.001	0.064
	O_{yl1}-H1	0.318	-1.644	-0.468	0.630
$INT5^{I}$	N1-H3	0.270	-1.286	-0.358	0.580
	O_{yl1}-H1	0.265	-1.160	-0.353	0.423
$INT6^{I}$	N1-H3	0.062	0.134	-0.008	0.316
	O_{yl1}-H1	0.260	-1.125	-0.344	0.405
$INT7^{I}$	N1-H3	0.056	0.130	-0.006	0.295
	O_{yl1}-H1	0.037	0.114	-0.001	0.083

Table S3 Electron density [ρ(r), au], its Laplacian [$\nabla^2\rho$(r), au], total energy density [H(r), au], and MBOs of the N-H and O_{yl1}-H bonds of the structures for pathway II

$NCCH_2N_2H_3$	bond	ρ(r)	$\nabla^2\rho$(r)	H(r)	MBOs
$IC1^{II}$	N1-H2	0.289	-1.414	-0.391	0.562
	O_{yl1}-H2	0.047	0.143	-0.002	0.187
$TS1^{II}$	N1-H2	0.129	-0.073	-0.081	0.315
	O_{yl1}-H2	0.180	-0.430	-0.188	0.346
$INT1^{II}$	N1-H2	0.040	0.104	-0.002	0.164
	O_{yl1}-H2	0.295	-1.425	-0.417	0.541
$IC2^{II}$	N1-H_w	0.035	0.096	-0.001	0.127
	O_{yl1}-H2	0.278	-1.286	-0.384	0.497
$INT2^{II}$	N1-H_w	0.281	-1.351	-0.376	0.574
	O_{yl1}-H2	0.038	0.119	-0.001	0.129
$IC3^{II}$	N1-H2	0.314	-1.612	-0.435	0.694
	O_{yl1}-H2	0.024	0.081	0.000	0.070
$TS3^{II}$	N1-H2	0.162	-0.345	-0.147	0.260
	O_{yl1}-H2	0.149	-0.154	-0.122	0.381
$INT3^{II}$	N1-H2	0.014	0.046	0.001	0.046
	O_{yl1}-H2	0.319	-1.646	-0.469	0.666
$INT4^{II}$	N2-H1	0.232	-0.961	-0.288	0.451
	O_{yl1}-H2	0.277	-1.283	-0.382	0.471
$INT5^{II}$	N2-H1	0.056	0.130	-0.006	0.243
	O_{yl1}-H2	0.275	-1.265	-0.377	0.461
$INT6^{II}$	N2-H1	0.052	0.127	-0.004	0.223
	O_{yl1}-H2	0.069	0.181	-0.009	0.182

Table S4 Electron density [ρ(r), au], its Laplacian [$\nabla^2\rho$(r), au], total energy density [H(r), au], and MBOs of the N-H and O_{yl1}-H bonds of the structures for pathway III

$NCCH_2N_2H_3$	bond	ρ(r)	$\nabla^2\rho$(r)	H(r)	MBOs
$IC1^{III}$	N1-H3	0.291	-1.433	-0.395	0.576
	O_{yl1}-H3	0.044	0.137	-0.001	0.162
$TS1^{III}$	N1-H3	0.133	-0.097	-0.087	0.325
	O_{yl1}-H3	0.177	-0.396	-0.180	0.330
$INT1^{III}$	N1-H3	0.046	0.115	-0.003	0.187
	O_{yl1}-H3	0.287	-1.351	-0.399	0.506
$IC2^{III}$	N1-H_w	0.048	0.124	-0.004	0.176
	O_{yl1}-H3	0.287	-1.389	-0.406	0.749
$TS2^{III}$	N1-H_w	0.089	0.112	-0.027	0.315
	O_{yl1}-H3	0.132	-0.044	-0.089	0.291
$INT2^{III}$	N1-H_w	0.290	-1.426	-0.393	0.611
	O_{yl1}-H3	0.037	0.113	-0.001	0.127
$IC3^{III}$	N1-H3	0.314	-1.613	-0.435	0.697
	O_{yl1}-H3	0.020	0.069	0.000	0.069
$TS3^{III}$	N1-H3	0.140	-0.162	-0.103	0.248
	O_{yl1}-H3	0.169	-0.345	-0.167	0.377
$INT3^{III}$	O_{yl1}-H3	0.321	-1.656	-0.471	0.724
$INT4^{III}$	N1-H1	0.220	-0.864	-0.266	0.444
	O_{yl1}-H3	0.291	-1.412	-0.412	0.533
$INT5^{III}$	N1-H1	0.061	0.133	-0.007	0.278
	O_{yl1}-H3	0.291	-1.411	-0.412	0.532
$INT6^{III}$	N1-H1	0.056	0.129	-0.005	0.261
	O_{yl1}-H3	0.057	0.163	-0.004	0.180

Table S5 Main atomic orbital (AO) composition (%) of LMOs of the structures for pathway I

$NCCH_2N_2H_3$	LMO number	Main AO composition of LMO (%)	Bonding assignment
$IC1^I$	34	$N2(2s(46.43)+2p_x(34.38))+H1(1s(18.77))$	σ(N2-H1)
	31	$O_{yl1}(2s(98.43))$	$Lp(O_{yl1})$
$TS1^I$	36	$N2(2s(62.60)+2p_x(27.94))+H1(1s(9.82))$	σ(N2-H1)
	65	$O_{yl1}(2p_z(13.93)+2p_x(60.49))+H1(1s(13.31))$	$\sigma(O_{yl1}$-H1)
$INT1^I$	36	$N2(2s(68.53)+2p_x(25.17))+H1(1s(6.14))$	σ(N2-H1)
	46	$O_{yl1}(2p_z(9.48)+2p_x(56.78))+H1(1s(20.70))$	$\sigma(O_{yl1}$-H1)
$IC3^I$	41	$O_w(2s(15.94)+2p_x(26.11)+2p_y(23.20)+2p_z(17.13))+H_w(1s(18.43))$	$\sigma(O_w$-$H_w)$
	36	$N2(2s(70.32)+2p_x(15.53)+2p_y(10.39))+H_w(1s(6.01))$	$\sigma(N2$-$H_w)$
$TS3^I$	39	$O_w(2s(22.74)+2p_x(17.85)+2p_y(20.50)+2p_z(28.55))+H_w(1s(13.63))$	$\sigma(O_w$-$H_w)$
	36	$N2(2s(60.38)+2p_x(24.32)+2p_y(9.07))+H_w(1s(8.90))$	$\sigma(N2$-$H_w)$
$INT3^I$	67	$O_w(2s(24.00)+2p_x(20.36)+2p_y(21.13)+2p_z(29.09))+H_w(1s(9.43))$	$\sigma(O_w$-$H_w)$
	36	$N2(2s(47.56)+2p_x(30.85))+H_w(1s(15.05))$	$\sigma(N2$-$H_w)$
$IC4^I$	34	$N2(2s(33.71)+2p_x(29.83))+H1(1s(23.79))$	σ(N2-H1)
	31	$O_{yl1}(2s(97.59))$	$Lp(O_{yl1})$
	24	$N1(2s(36.78)+2p_x(34.80))+H2(1s(20.96))$	σ(N1-H2)
	64	$O_w(2s(7.95)+2p_x(82.63))+H2(1s(4.46))$	$\sigma(O_w$-H2)
$TS4^I$	34	$N2(2s(44.61)+2p_x(28.09))+H1(1s(17.83))$	σ(N2-H1)
	31	$O_{yl1}(2s(97.97))$	$Lp(O_{yl1})$
	25	$N1(2s(64.53)+2p_x(24.36))+H2(1s(5.26))$	σ(N1-H2)
	48	$O_w(2s(16.18)+2p_x(64.95))+H2(1s(16.80))$	$\sigma(O_w$-H2)
$INT4^I$	36	$N2(2s(68.14)+2p_x(20.13))+H1(1s(1.06))$	σ(N2-H1)
	46	$O_{yl1}(2p_z(10.80)+2p_x(51.06))+H1(1s(26.98))$	$\sigma(O_{yl1}$-H1)
	37	$N1(2s(46.63)+2p_x(31.18))+H2(1s(15.96))$	σ(N1-H2)
	62	$O_w(2s(14.95)+2p_x(79.26))+H2(1s(8.13))$	$\sigma(O_w$-H2)
$INT5^I$	25	$N1(2s(45.01)+2p_x(13.21)+2p_y(16.86)+2p_z(10.56))+H3(1s(17.10))$	σ(N1-H3)

	61	O_w(2s(15.42)+2p_x(44.49)+2p_y(12.71)+2p_z(21.69))+H3(1s(6.94))	σ(O_w-H3)
	52	O_{yl1}(2p_x(26.22)+2p_y(43.88))+H1(1s(19.73))	σ(O_{yl1}-H1)
	76	Ow(2p_y(52.90)+2p_z(28.52))+H_w(1s(4.91))	σ(O_w-H_w)
$INT6^I$	27	N1(2s(62.55)+2p_x(13.24)+2p_y(18.60))+H3(1s(6.09))	σ(N1-H3)
	41	O_w(2s(13.33)+2p_x(42.04)+2p_y(17.61))+H3(1s(17.91))	σ(O_w-H3)
	52	O_{yl1}(2p_y(67.48))+H1(1s(19.33))	σ(O_{yl1}-H1)
	75	O_w(2p_x(46.34)+2p_y(13.58)+2p_z(27.73))+H_w(1s(5.71))	σ(O_w-H_w)
$INT7^I$	28	N1(2s(63.04)+2p_y(18.29)+2p_z(10.51))+H3(1s(5.60))	σ(N1-H3)
	41	O_w(2s(12.72)+2p_x(31.26)+2p_y(19.86)+2p_z(17.78))+H3(1s(18.64))	σ(O_w-H3)
	37	O_{yl1}(2s(99.55))	Lp(O_{yl1})
	44	O_w(2s(14.81)+2p_x(15.42)+2p_z(49.14))+H_w(1s(17.16))	σ(O_w-H_w)

Table S6 Main atomic orbital (AO) composition (%) of LMOs of the structures for pathway II

$NCCH_2N_2H_3$	LMO number	Main AO composition of LMO (%)	Bonding assignment
$IC1^{II}$	24	N1(2s(42.71)+2p_x(30.78))+H2(1s(19.15))	σ(N1-H2)
	31	O_{yl1}(2s(98.21))	Lp(O_{yl1})
$TS1^{II}$	26	N1(2s(59.49)+2p_x(27.87))+H2(1s(8.96))	σ(N1-H2)
	65	O_{yl1}(2p_z(29.87)+2p_x(43.95))+H2(1s(13.82))	σ(O_{yl1}-H2)
$INT1^{II}$	29	N1(2s(65.96)+2p_x(32.25))+H2(1s(2.87))	σ(N1-H2)
	45	O_{yl1}(2p_z(21.75)+2p_x(41.21))+H2(1s(24.32))	σ(O_{yl1}-H2)
$IC3^{II}$	24	N1(2s(33.85)+2p_x(38.29))+H2(1s(22.17))	σ(N1-H2)
	31	O_{yl1}(2s(97.84))	Lp(O_{yl1})
$TS3^{II}$	24	N1(2s(63.09)+2p_x(23.25))+H2(1s(7.82))	σ(N1-H2)
	30	O_{yl1}(2s(98.98))+H2(1s(1.31))	σ(O_{yl1}-H2)
$INT3^{II}$	23	N1(2s(66.69)+2p_x(26.43))	Lp(N1)
	46	O_{yl1}(2p_z(12.10)+2p_x(50.45))+H2(1s(27.38))	σ(O_{yl1}-H2)

Table S7 Main atomic orbital (AO) composition (%) of LMOs of the structures for pathway III

$NCCH_2N_2H_3$	LMO number	Main AO composition of LMO (%)	Bonding assignment
$IC1^{III}$	24	N1(2s(42.60)+2p_x(27.90))+H3(1s(19.87))	σ(N1-H3)
	31	O_{yl1}(2s(98.25))	Lp(O_{yl1})
$TS1^{III}$	25	N1(2s(63.03)+2p_x(23.52))+H3(1s(8.47))	σ(N1-H3)
	64	O_{yl1}(2p_y(25.74)+2p_x(39.26))+H3(1s(14.10))	σ(O_{yl1}-H3)
$INT1^{III}$	28	N1(2s(67.85)+2p_x(24.08))+H3(1s(3.47))	σ(N1-H3)
	45	O_{yl1}(2p_y(20.18)+2p_x(37.39))+H3(1s(22.94))	σ(O_{yl1}-H3)
$IC2^{III}$	48	O_{yl1}(2p_x(53.39)+2p_z(13.90))+H3(1s(22.40))	σ(O_{yl1}-H3)
	29	N1(2s(70.54)+2p_x(20.80)+2p_y(8.78))+H_w(1s(4.60))	σ(N1-H_w)
$TS2^{III}$	33	O_{yl1}(2s(90.90))	Lp(O_{yl1})
	28	N1(2s(65.14)+2p_x(18.41)+2p_y(7.76))+H_w(1s(7.25))	σ(N1-H_w)
$INT2^{III}$	35	O_{yl1}(2s(93.90))	Lp(O_{yl1})
	40	N1(2s(43.26)+2p_x(32.17)+2p_y(8.02))+H_w(1s(19.45))	σ(N1-H_w)
$IC3^{III}$	38	N1(2s(33.58)+2p_x(28.60))+H3(1s(23.21))	σ(N1-H3)
	36	O_{yl1}(2s(97.68))	Lp(O_{yl1})
$TS3^{III}$	24	N1(2s(64.42)+2p_x(20.56))+H3(1s(6.73))	σ(N1-H3)
	30	O_{yl1}(2s(99.02))+H3(1s(1.36))	σ(O_{yl1}-H3)
$INT3^{III}$	23	N1(2s(69.54)+2p_z(20.12))	Lp(N1)
	46	O_{yl1}(2p_y(40.63)+2p_z(14.23))+H3(1s(28.86))	σ(O_{yl1}-H3)

Table S8 Selected spin density on the Np, O, and N atoms (atomic units) of the IC, TS, and INT of pathway I.

Complexes	Np	O_{yl1}	O_{yl2}	N1	N2
$IC1^{I}$	2.242	-0.105	-0.145	-0.448	-0.560
$TS1^{I}$	2.260	-0.096	-0.161	-0.376	-0.625
$INT1^{I}$	2.269	-0.090	-0.175	-0.330	-0.662
$IC2^{I}$	2.247	-0.092	-0.159	0.358	0.611
$INT2^{I}$	2.244	-0.107	-0.140	0.358	0.629
$IC3^{I}$	2.243	-0.108	-0.138	0.352	0.638
$TS3^{I}$	2.232	-0.108	-0.131	0.381	0.616
$INT3^{I}$	2.254	-0.112	-0.129	0.436	0.569
$IC4^{I}$	1.420	-0.071	-0.083	0.407	0.413
$TS4^{I}$	2.152	-0.084	-0.120	0.031	0.016
$INT4^{I}$	2.296	-0.087	-0.203	0.000	0.000
$INT5^{I}$	2.308	-0.102	-0.179	0.000	0.000
$INT6^{I}$	2.295	-0.110	-0.169	0.000	-0.001
$INT7^{I}$	2.249	-0.121	-0.133	0.000	0.000

Table S9 Selected spin density on the Np, O, and N atoms (atomic units) of the IC, TS, and INT of pathway II.

Complexes	Np	O_{yl1}	O_{yl2}	N1	N2
$IC1^{II}$	2.244	-0.099	-0.149	-0.496	-0.513
$TS1^{II}$	2.261	-0.088	-0.174	-0.558	-0.450
$INT1^{II}$	2.278	-0.091	-0.196	-0.559	-0.423
$IC2^{II}$	2.266	-0.082	-0.181	0.577	0.405
$INT2^{II}$	2.246	-0.097	-0.137	0.504	0.504
$IC3^{II}$	1.200	-0.061	-0.076	0.423	0.572
$TS3^{II}$	2.073	-0.073	-0.138	0.116	0.104
$INT3^{II}$	2.285	-0.077	-0.204	0.000	0.000
$INT4^{II}$	2.282	-0.089	-0.174	0.000	0.000
$INT5^{II}$	2.264	-0.094	-0.180	0.000	0.000
$INT6^{II}$	2.255	-0.118	-0.137	0.000	0.000

Table S10 Selected spin density on the Np, O, and N atoms (atomic units) of the IC, TS, and INT of pathway III.

Complexes	Np	O_{yl1}	O_{yl2}	N1	N2
$IC1^{III}$	2.248	-0.110	-0.142	-0.485	-0.525
$TS1^{III}$	2.261	-0.107	-0.163	-0.504	-0.483
$INT1^{III}$	2.271	-0.104	-0.177	-0.539	-0.440
$IC2^{III}$	2.545	-0.085	-0.176	0.519	0.228
$TS2^{III}$	2.241	-0.096	-0.148	0.632	0.386
$INT2^{III}$	2.231	-0.107	-0.135	0.537	0.484
$IC3^{III}$	1.173	-0.059	-0.079	0.481	0.537
$TS3^{III}$	1.834	-0.072	-0.141	0.216	0.184
$INT3^{III}$	2.293	-0.069	-0.222	0.000	0.000
$INT4^{III}$	2.257	-0.088	-0.184	0.000	0.000
$INT5^{III}$	2.278	-0.094	-0.182	0.000	0.000
$INT6^{III}$	2.266	-0.107	-0.157	0.000	0.000

Cartesian coordinates and energies of Pathway I

IC1[I]

Atom	X	Y	Z (Angstrom)
Np	-0.81660000	0.04980000	-0.09050000
O	-0.76040000	-2.69330000	-1.01210000
H	-0.42850000	-3.46120000	-0.51710000
O	-2.61580000	-1.21850000	1.41620000
H	-2.20780000	-1.20640000	2.30000000
O	-1.86340000	1.79930000	1.72670000
H	-2.72850000	1.99390000	1.32500000
O	0.10580000	2.44870000	-0.60670000
H	1.07200000	2.50470000	-0.47560000
O	0.98990000	-0.83900000	-2.02420000
H	0.51550000	-1.69220000	-1.88530000
H	0.57150000	-0.46570000	-2.81880000
H	-1.44330000	-3.05180000	-1.60390000
H	-3.34610000	-0.57880000	1.48850000
H	-2.08020000	1.18000000	2.44570000
H	-0.02000000	2.59230000	-1.56050000
O	0.49580000	-0.25050000	1.20700000
O	-2.11080000	0.34120000	-1.35840000
N	3.59700000	-1.91670000	1.30660000
N	3.15670000	-0.74240000	0.89140000
H	4.60550000	-2.06690000	1.30310000
H	3.04260000	-2.36070000	2.03620000
H	2.11790000	-0.57060000	0.97990000
C	3.92910000	-0.03750000	-0.12380000
H	4.99330000	-0.07160000	0.13360000
H	3.79070000	-0.50850000	-1.10590000
C	3.48360000	1.35260000	-0.19610000
N	3.11490000	2.45060000	-0.26950000

E = -1290.5068343 a.u.

TS1[I]

Atom		X	Y	Z (Angstrom)
Np	-0.808082	-0.039291	0.099579	
O	-0.715676	2.638039	1.088202	
H	-0.518131	3.327723	0.432255	
O	-2.439213	1.191918	-1.495489	
H	-1.990355	1.187328	-2.360019	
O	-1.822851	-1.814537	-1.727432	
H	-2.757064	-1.839875	-1.453803	
O	0.124579	-2.390716	0.665169	
H	1.084112	-2.472507	0.493213	
O	1.011681	0.694265	2.025631	
H	0.574246	1.573288	2.009403	
H	0.629997	0.250508	2.802880	
H	-1.576368	2.889075	1.463724	
H	-3.171015	0.558677	-1.607925	
H	-1.829820	-1.225915	-2.503181	
H	0.041133	-2.466653	1.632148	
O	0.566058	0.258636	-1.242955	
O	-2.108372	-0.322624	1.339390	
N	3.424906	1.997253	-1.154274	
N	2.991543	0.767814	-0.880502	
H	4.430463	2.166932	-1.126497	
H	2.913341	2.464672	-1.897709	
H	1.687524	0.493813	-1.034150	
C	3.859643	0.033047	0.028482	
H	4.902057	0.050197	-0.318018	
H	3.835210	0.467768	1.037658	
C	3.415575	-1.357843	0.113478	
N	3.057168	-2.459638	0.191536	

E = -1290.5046454 a.u.

INT1[1]

Atom	X	Y	Z (Angstrom)
Np	-0.85619200	-0.06401800	0.08044300
O	-0.81672900	2.67811700	0.94674200
H	-0.61228400	3.20918200	0.15835100
O	-2.46115000	1.17308200	-1.53679400
H	-2.08077500	1.03154600	-2.42242800
O	-2.00766100	-1.85269600	-1.42692300
H	-2.85089600	-2.02996500	-0.97322100
O	0.35455000	-2.20536500	0.84869300
H	1.24915700	-2.31139700	0.46847700
O	0.96082900	0.81687900	1.97308000
H	0.47965100	1.67037600	1.92389900
H	0.59323200	0.37987800	2.76090400
H	-1.74139600	2.89310000	1.15637400
H	-3.28487200	0.65325100	-1.54479800
H	-2.26954700	-1.38174800	-2.23816600
H	0.50477800	-2.11255500	1.80615700
O	0.53392400	0.22844600	-1.33024400
O	-2.14205200	-0.33422600	1.32851500
N	3.60535200	2.07248300	-0.88484900
N	3.15270400	0.81278900	-0.79198800
H	4.61513000	2.22335800	-0.86251200
H	3.11021700	2.62957500	-1.57440300
H	1.49191700	0.44151200	-1.04907200
C	4.07756900	-0.01488100	-0.02839200
H	5.09149300	-0.00118300	-0.45704600
H	4.15997700	0.32777000	1.01386800
C	3.59799400	-1.39662000	-0.01934100
N	3.20522800	-2.49011500	-0.00683200

E = -1290.5066098 a.u.

IC2[1]

Atom	X	Y	Z (Angstrom)
Np	-1.25646600	-0.08931100	-0.12659200
O	-3.37203900	0.66935900	1.12936600
H	-3.12429800	1.38887300	1.73691900
O	-0.61895000	2.45202600	-0.44478400
H	-0.82862800	2.75176400	-1.34790300
O	1.98859500	3.05334900	0.52660900
H	2.63922000	2.82943800	-0.16538600
O	0.86909100	-0.77711800	-1.36918500
H	1.64690100	-0.98891600	-0.78796800
H	0.71013700	-1.58087100	-1.89429100
H	-3.97172000	1.08502400	0.48446600
H	-1.21184800	2.96662800	0.13360200
H	1.11425300	2.91111700	0.10047300
O	-0.34411500	-0.10921000	1.63266100
O	-2.21358800	-0.11738500	-1.65340900
N	3.38176500	-2.58648600	0.64419900
N	3.23150800	-1.34916000	0.15406900
H	4.29015000	-2.86434700	1.01804300
H	2.57667100	-2.92712400	1.16012800
H	0.62068400	0.26698700	1.72861800
C	4.51104800	-0.81749900	-0.31293900
H	5.26904800	-0.82457400	0.48609800
H	4.91297800	-1.40696300	-1.15006100
C	4.31871000	0.56416100	-0.75951700
N	4.14623500	1.66150400	-1.09816900
O	2.05775200	0.72918800	1.93856500
H	2.08606800	1.59024400	1.43306200
H	2.49910100	0.07329600	1.35631200
O	-1.65872300	-2.63429500	0.14555200
H	-1.84434100	-2.81023500	1.08510100
H	-2.49234400	-2.84271200	-0.31314900

E = -1366.936520 a.u.

INT2[1]

Atom	X	Y	Z (Angstrom)
Np	-1.27493500	-0.16318800	-0.07691600
O	-3.39266200	0.62623700	1.22491400
H	-3.08877000	1.22647900	1.92841600
O	-0.87553500	2.56456000	-0.07111100
H	-1.19829000	2.92411800	-0.91617800
O	1.80683500	2.89321600	0.47652600
H	2.27801300	2.72187700	-0.36286100
O	0.87547300	-0.90586200	-1.34590900
H	1.51233100	-1.13388800	-0.64573000
H	0.68376200	-1.75334200	-1.78515200
H	-3.88937900	1.20132500	0.61717800
H	-1.45584400	2.95946600	0.60405100
H	0.84626400	2.88102400	0.23625500
O	-0.32927800	-0.46570000	1.50123300
O	-2.21977200	0.12233300	-1.61361100
N	4.37155300	-1.93975000	1.21030300
N	3.87024900	-0.84589400	0.62418000
H	5.31895800	-2.23108400	0.96537800
H	4.13732600	-2.01935100	2.19524400
H	1.10580300	0.24338100	1.64831800
C	4.47857900	-0.60339500	-0.67812100
H	5.57207700	-0.50115200	-0.60132600
H	4.27435600	-1.42634500	-1.37826700
C	3.93358200	0.63376600	-1.24074200
N	3.49407100	1.61813700	-1.67239300
O	2.01348400	0.69530800	1.76372100
H	1.96554000	1.60006300	1.23654500
H	2.72040900	0.08888100	1.31350600
O	-1.68691600	-2.74194300	-0.35015900
H	-1.80383800	-3.09459700	0.54961200
H	-2.56687200	-2.82525300	-0.75805400

E = -1366.950282 a.u.

IC3^{I}

Atom	X	Y	Z (Angstrom)
Np	-1.26062800	-0.16160600	-0.06997700
O	-3.37482800	0.63108600	1.23727400
H	-3.06392800	1.21281000	1.95322100
O	-0.86593000	2.56701900	-0.06708100
H	-1.21975500	2.93081600	-0.89779800
O	1.82857600	2.90630400	0.39713700
H	2.28125900	2.69349900	-0.44281500
O	0.86407900	-0.94178400	-1.36453500
H	1.35239800	-1.52863400	-0.76155800
H	0.57042000	-1.52570300	-2.08589600
H	-3.86065000	1.22553900	0.63943100
H	-1.41841400	2.96044200	0.63188800
H	0.86316000	2.89013900	0.17757100
O	-0.29867800	-0.45411500	1.49720800
O	-2.21144700	0.12179700	-1.60343100
N	4.45859400	-1.82019800	1.30074300
N	3.94197600	-0.74658700	0.68982900
H	5.31179600	-2.22836200	0.91578900
H	4.42534900	-1.76774600	2.31428600
H	1.14793400	0.28455000	1.64468300
C	4.25717700	-0.73193900	-0.73293300
H	5.33751300	-0.84067600	-0.91253800
H	3.75122200	-1.55124200	-1.26412600
C	3.81491700	0.53827400	-1.31242700
N	3.46196700	1.55062700	-1.75881500
O	2.04191500	0.75469300	1.76407100
H	1.98848500	1.64137200	1.20991400
H	2.78047000	0.15114400	1.34435500
O	-1.73313000	-2.75598400	-0.27050500
H	-1.86707600	-3.05827000	0.64510600
H	-2.61651700	-2.81739600	-0.67487100

E = -1366.950531 a.u.

TS3^{I}

Atom	X	Y	Z (Angstrom)
Np	-1.25008500	-0.14774800	-0.07370900
O	-3.36342900	0.64409800	1.23858800
H	-3.04807500	1.20951200	1.96562700
O	-0.81676200	2.56908800	-0.04965100
H	-1.17417100	2.95197500	-0.87001800
O	1.89740500	2.94878900	0.44273500
H	2.35441300	2.74002500	-0.39389100
O	0.87673100	-0.91773700	-1.37615300
H	1.27842600	-1.64492600	-0.86986700
H	0.57835000	-1.33436200	-2.20380000
H	-3.84263400	1.25380400	0.65093800
H	-1.36167400	2.95232900	0.66084300
H	0.93690000	2.90933900	0.21760000
O	-0.30724000	-0.47465800	1.49046200
O	-2.19262600	0.15639700	-1.61022100
N	4.11559300	-1.93588100	1.31055500
N	3.81473100	-0.79668400	0.69098400
H	4.91141200	-2.47362100	0.96778400
H	3.99268600	-1.90815200	2.31912000
H	1.21991500	0.25896100	1.66182800
C	4.19083900	-0.76480100	-0.71548500
H	5.27022500	-0.93277300	-0.83671800
H	3.66363800	-1.54461300	-1.28190900
C	3.84445200	0.53919600	-1.28300700
N	3.56533000	1.57465000	-1.72770100
O	2.12039500	0.68460700	1.77706100
H	2.07081900	1.56816700	1.27210000
H	2.91933200	-0.01375400	1.23861100
O	-1.68931800	-2.72784100	-0.33586500
H	-1.82746800	-3.06206700	0.56793800
H	-2.56674900	-2.79219300	-0.75276200

E = -1366.949284 a.u.

INT3[I]

Atom	X	Y	Z (Angstrom)
Np	-1.27170300	-0.15022200	-0.06739400
O	-3.38515000	0.64580600	1.24578400
H	-3.06735300	1.21846400	1.96605800
O	-0.80688600	2.55520100	-0.03854200
H	-1.17907200	2.93038400	-0.85593600
O	1.92453800	3.02151700	0.39278300
H	2.36141200	2.76266900	-0.43907500
O	0.84779900	-0.93966900	-1.37313500
H	1.22520200	-1.68425000	-0.87335200
H	0.55253200	-1.33524100	-2.21211100
H	-3.86374300	1.25042400	0.65236500
H	-1.34629800	2.93787400	0.67651300
H	0.96267700	2.94563700	0.19425500
O	-0.33857700	-0.48744000	1.49137200
O	-2.21045900	0.16326500	-1.60619000
N	4.43216900	-1.82538000	1.34745700
N	3.99316500	-0.78633800	0.65670700
H	5.23427700	-2.33211700	0.97401200
H	4.34560300	-1.74182500	2.35813500
H	1.28774200	0.27974700	1.69358800
C	4.18174300	-0.80698000	-0.78714900
H	5.23440300	-1.00451900	-1.02268400
H	3.57099800	-1.59488700	-1.24630600
C	3.79475400	0.48664700	-1.34939900
N	3.48723000	1.51096900	-1.79934800
O	2.16902400	0.70484300	1.82675300
H	2.11237400	1.56001700	1.31682800
H	3.22276600	-0.17656900	1.12217300
O	-1.81969000	-2.74114200	-0.26648400
H	-1.97649400	-3.02813800	0.65028400
H	-2.70039500	-2.76884700	-0.68023600

E = -1366.951950 a.u.

IC4[I]

Atom	X	Y	Z (Angstrom)
Np	-0.99490100	-0.16404400	0.02217700
O	-1.91048800	1.77091600	-1.31960000
H	-1.73091500	1.71370900	-2.27584500
O	-1.90348800	-2.07024300	-1.34229000
H	-2.87289500	-2.10790300	-1.25037400
O	0.40224800	-2.23905300	1.27705700
H	0.15286900	-2.37667100	2.20857600
O	0.18982900	1.40913000	1.62663600
H	0.02141100	2.29266200	1.17152700
O	-0.45329300	3.62622500	0.27640800
H	-1.01785400	3.13993300	-0.36335700
H	-1.08983600	4.06366100	0.86823500
H	-2.87817400	1.85223000	-1.23366100
H	-1.74081300	-1.92206500	-2.29165800
H	0.15169100	-3.06595000	0.82630800
H	-0.37676600	1.42831200	2.41879800
O	0.41520800	-0.14213400	-1.02188800
O	-2.40217000	-0.18777800	1.05265900
N	3.07810900	-1.59152400	0.75506700
N	3.18904700	-1.02886300	-0.43544000
H	2.30619677	-0.64754851	-0.80404378
C	4.45093300	-0.43858800	-0.86614300
H	5.27951700	-1.05045300	-0.49839900
H	2.06576145	-1.94444522	1.03953791
H	3.92177700	-2.00356100	1.15248000
H	4.46827700	-0.44758900	-1.95909100
C	4.59883400	0.94427400	-0.39019500
N	4.70403600	2.04051700	-0.02094800

E = -1290.3294053 a.u.

TS4^{I}

Atom	X	Y	Z (Angstrom)
Np	-0.90608600	-0.18355100	0.02141600
O	-1.75301100	1.92802100	-1.21998300
H	-1.37481700	1.99751600	-2.11456200
O	-2.11141900	-1.78318000	-1.58046700
H	-3.07304600	-1.67724600	-1.47119800
O	0.63216300	-2.87769300	1.08093600
H	0.63350500	-3.31460900	1.96195200
O	0.22627400	1.31516800	1.76963000
H	0.00398400	2.22826900	1.41768000
O	-0.56281900	3.64749800	0.67883600
H	-1.03647100	3.19270600	-0.05324500
H	-1.27398700	3.91272600	1.28754100
H	-2.71819300	1.98774900	-1.33608900
H	-1.93667300	-1.54243600	-2.50753900
H	0.43060000	-3.57353400	0.41628900
H	-0.33236800	1.21973500	2.56067700
O	0.52489400	-0.07398500	-1.07264200
O	-2.33246300	-0.27380400	1.07662800
N	2.97278500	-1.87440500	0.54076500
N	3.02919700	-0.86827300	-0.22826400
H	2.10887200	-0.51186800	-0.58101600
C	4.26517600	-0.20415200	-0.66357600
H	5.11091700	-0.58728400	-0.08540500
H	1.61173900	-2.50488000	0.88398300
H	3.90190100	-2.18122500	0.85577600
H	4.42156800	-0.43592500	-1.72504700
C	4.14336600	1.24425600	-0.49543800
N	4.04776900	2.39464200	-0.37119600

E = -1290.3004755 a.u.

INT4[I]

Atom	X	Y	Z (Angstrom)
Np	-0.99883400	-0.21241300	0.02803100
O	-2.16870400	2.00913200	-0.89564000
H	-2.06875100	2.08710200	-1.86130000
O	-2.21831000	-1.81003600	-1.56953500
H	-3.17889600	-1.70069100	-1.45297100
O	0.74553600	-2.65857800	0.93112000
H	0.63425500	-3.09008900	1.79829800
O	0.18600600	1.31674000	1.70201100
H	0.03219500	2.23009900	1.31411200
O	-0.39876300	3.65467900	0.51367200
H	-1.09999200	3.22499900	-0.02785500
H	-0.89288700	4.14138000	1.19574300
H	-3.12675500	2.05835000	-0.73029700
H	-2.04754800	-1.52595300	-2.48545800
H	0.57138700	-3.36263700	0.27958300
H	-0.36207400	1.29558100	2.50590500
O	0.45583600	0.06597500	-1.37056200
O	-2.40029400	-0.36177400	1.15595100
N	3.21882400	-1.81066300	0.59390400
N	3.29174400	-0.83384800	-0.14895100
H	1.35195500	-0.08292100	-0.99131000
C	4.63794900	-0.31240800	-0.40862400
H	5.36546600	-0.62696000	0.34808200
H	2.23158400	-2.23120200	0.77099300
H	4.06040100	-2.22438900	1.03530000
H	4.93130100	-0.73845900	-1.38015200
C	4.58683700	1.14271300	-0.51966300
N	4.56524700	2.30012300	-0.60094500

E = -1290.3374676 a.u.

INT5[I]

Atom	X	Y	Z (Angstrom)
Np	-0.93199600	-0.38579800	-0.02011100
O	1.14021700	1.78035200	-1.16583400
H	1.14069400	2.64550000	-0.71789300
O	2.65923900	-2.68838000	-1.19158300
H	3.53589100	-2.83384700	-0.79385100
O	-3.01437200	-1.66974800	0.78058000
H	-2.99702800	-2.54884700	0.36167900
O	-3.38518600	1.57731800	-0.65125600
H	-2.63809600	1.66007800	-1.30355000
O	-1.33032800	1.64609200	-2.45750400
H	-0.47405500	1.74791100	-1.97466500
H	-1.31692600	0.71123000	-2.72965200
H	1.66051300	1.93484700	-1.97523800
H	2.81394700	-1.97590600	-1.83637700
H	-2.92175500	-1.84875300	1.73345700
H	-4.14573600	2.00018700	-1.08419800
O	-0.91994000	0.62040300	1.69650500
O	-0.90674800	-1.37876300	-1.52751200
N	2.82948400	0.03179100	2.11350000
N	3.70074800	0.71694600	1.57334500
H	-1.53063400	1.45732900	1.71470500
C	3.80329900	0.54110100	0.12558600
H	3.65044600	-0.50117100	-0.17680600
H	2.19146400	-0.66771300	1.59333300
H	2.98148300	1.13562100	-0.31783800
C	5.08539900	1.04178600	-0.35699000
N	6.09585100	1.43214400	-0.77383400
H	2.71335000	0.16587000	3.12620900
O	1.19558400	-1.64170000	0.75772800
H	0.95174500	-2.37493800	1.35370500
H	1.73682900	-2.05378700	0.00974600
O	-2.47957900	2.69592300	1.61434900
H	-3.16451700	2.52762900	2.28513300
H	-2.89781600	2.40246300	0.75602300

E = -1443.215503 a.u.

INT6[1]

Atom	X	Y	Z (Angstrom)
Np	1.14767000	-0.50866700	-0.08493900
O	-1.09044600	1.19585200	1.32514300
H	-1.45469000	2.07774200	1.13150000
O	-2.10267400	-2.08897600	1.43382600
H	-2.80901000	-2.74781700	1.56805900
O	3.61863100	-1.07297500	-0.39128300
H	3.78575400	-1.93917000	0.02113400
O	3.21493100	2.64283700	0.48158600
H	2.59750700	2.30711700	1.18339000
O	1.49210100	1.60714900	2.33325700
H	0.57234000	1.49483700	1.99003800
H	1.79197000	0.69713300	2.50076000
H	-1.55920300	0.91790100	2.13210900
H	-2.47847200	-1.25064600	1.76009800
H	3.81535700	-1.20224700	-1.33654500
H	3.53871200	3.49160000	0.82787700
O	1.14019600	0.50032900	-1.78136600
O	1.16612400	-1.52211900	1.38987500
N	-3.42556100	-0.01053000	-2.01340600
N	-4.26197500	0.68659500	-1.42307700
H	1.22444300	1.53166900	-1.66836400
C	-4.31469200	0.38935000	0.02734000
H	-4.17375000	-0.67631900	0.23233400
H	-2.39860200	-1.12629700	-1.41797900
H	-3.49398200	0.94081700	0.50328000
C	-5.58524800	0.83951500	0.58939900
N	-6.59246300	1.18453400	1.05335800
H	-3.40471500	0.25307300	-3.00955000
O	-1.68870300	-1.78008600	-1.02538900
H	-1.79053700	-2.64250100	-1.48023800
H	-1.90120700	-1.92958600	0.00833300
O	1.36039500	3.05322700	-1.40845500
H	1.79251200	3.41165900	-2.20350900
H	2.08742400	3.01778300	-0.71954200

E = -1443.199138 a.u.

INT7[I]

Atom	X	Y	Z (Angstrom)
Np	0.95925800	-0.44787900	-0.00086600
O	-0.84309600	1.92886300	0.99329500
H	-0.93865000	2.77199900	0.51581400
O	-2.46158000	-2.42431800	1.82863200
H	-3.14635800	-3.11815800	1.86909300
O	3.05419000	-1.70573000	-0.81290400
H	3.22602400	-2.44146500	-0.19958500
O	3.42105400	2.25144300	0.41396400
H	2.64708500	2.12625400	1.14628700
O	1.64078200	1.91648800	2.14280900
H	0.74268300	1.95981700	1.71171000
H	1.72677900	0.97591700	2.39571900
H	-1.43625500	2.02062300	1.76012100
H	-2.92676900	-1.60579800	2.08275400
H	2.89253500	-2.13064700	-1.67376700
H	3.88657400	3.08756100	0.61818900
O	0.61272000	0.20506000	-1.67974700
O	1.31527400	-1.07058800	1.67075800
N	-3.10097200	-0.35699900	-1.92174500
N	-3.79355600	0.60579200	-1.56356900
H	1.63900800	1.66498200	-1.81290200
C	-3.91654200	0.69089600	-0.09130400
H	-3.84442800	-0.29162300	0.38573800
H	-2.26605900	-1.50156600	-1.03471200
H	-3.07983900	1.30866100	0.26138500
C	-5.17144600	1.34114300	0.27622200
N	-6.16663300	1.85347000	0.58628900
H	-3.01666200	-0.34705500	-2.94913800
O	-1.67146500	-2.17179000	-0.52091300
H	-1.73932300	-3.03767600	-0.97493400
H	-2.05466100	-2.28918300	0.48038800
O	2.25196700	2.44598500	-1.82221100
H	2.91789500	2.22416800	-2.49804300
H	2.95676200	2.36457900	-0.52939500

E = -1443.202243 a.u.

IC5[I]

Atom	X	Y	Z (Angstrom)
N	1.42352300	-0.96747300	-0.00003100
N	1.38567100	0.26762900	-0.00000400
C	0.08245700	0.99993800	0.00001700
H	0.08870600	1.64970900	0.88029400
H	0.47588800	-1.41013900	-0.00003300
H	0.08869300	1.64973500	-0.88024200
C	-1.11598600	0.16627200	0.00001300
N	-2.01663900	-0.56966500	0.00000700

E = -242.198881 a.u.

TS5[I]

Atom	X	Y	Z (Angstrom)
N	-1.26716700	-0.84130000	0.00009600
N	-1.31926900	0.32445100	-0.00000400
C	0.32473300	1.25449800	-0.00020000
H	0.25749300	1.83901300	-0.91552100
H	-0.09332600	-1.28223800	0.00066200
H	0.25804400	1.84051000	0.91422800
C	1.16216900	0.15908300	0.00072000
N	1.25163200	-1.03726100	-0.00044700

E = -242.174490 a.u.

INT8[I]

Atom	X	Y	Z (Angstrom)
N	-2.32492000	0.42211300	0.00010600
N	-2.03200400	-0.64382900	-0.00034300
C	1.56012000	-1.17346000	0.00016400
H	1.62468800	-1.71957900	0.93639000
H	0.36818000	1.74288900	0.00028100
H	1.62422600	-1.71978700	-0.93597100
C	1.37816400	0.12584400	0.00007500
N	1.32166700	1.36202700	-0.00006700

E = -242.239272 a.u.

IC6[I]

Atom	X	Y	Z (Angstrom)
C	-2.10179000	0.60298400	0.00083800
H	-2.38220700	1.08365800	0.93320500
H	0.29756600	-1.42861200	-0.03562400
H	-2.46974100	1.00965900	-0.93631000
C	-1.36712500	-0.49180800	0.00933800
N	-0.73818400	-1.54976800	0.02001000
O	2.06509900	-0.86489100	-0.10851900
H	1.78257200	0.08466200	-0.11921000
H	2.29232900	-1.01959100	0.82353700
O	1.07281300	1.73864100	-0.09200400
H	0.12675800	1.48925900	-0.10124000
H	1.23020300	1.97229400	0.83869600

E = -285.579143 a.u.

TS6[I]

Atom	X	Y	Z (Angstrom)
C	-1.69888200	0.83497800	-0.00527300
H	-2.12491700	1.23197000	0.91543200
H	0.74906700	-1.27850100	-0.04304500
H	-2.16805500	1.18911800	-0.92257100
C	-1.31139300	-0.48389500	0.01618400
N	-0.82222800	-1.57398300	0.02704400
O	1.71609600	-0.86581700	-0.10959800
H	1.51929400	0.22004700	-0.08546500
H	2.17028900	-1.09245600	0.72583400
O	1.07460400	1.53544100	-0.08814600
H	0.04889100	1.39281100	-0.05413300
H	1.29708300	1.89140400	0.79113600

E = -285.556485 a.u.

INT9[I]

Atom	X	Y	Z (Angstrom)
C	-2.28929300	0.43021600	-0.09864700
H	-2.88138100	0.51083700	0.81794300
H	1.45486700	-1.16782100	-0.09859700
H	-2.95500700	0.21785100	-0.94065700
C	-1.30514400	-0.63117300	0.03610800
N	-0.51475600	-1.47760400	0.14026500
O	2.31168100	-0.70422200	-0.19312500
H	1.50299300	0.94619400	-0.10779900
H	2.67542100	-0.72369700	0.70823100
O	1.00347400	1.79001600	-0.00554800
H	-1.76766500	1.37512900	-0.27780700
H	0.61944200	1.70412400	0.88145600

E = -285.621208 a.u.

Cartesian coordinates and energies of Pathway II

$IC1^{II}$

Atom	X	Y	Z (Angstrom)
Np	-1.01772600	-0.25200500	-0.04947700
O	-1.05055100	-2.47098800	1.33218900
H	-1.61784300	-3.08473800	0.83337100
O	-2.51417200	0.95718400	1.74587000
H	-1.87565000	1.34886600	2.36612700
O	-3.14137800	2.98846800	-0.00199000
H	-4.01620300	2.97284900	-0.42747600
O	-1.01021100	1.96642000	-1.39322400
H	-0.24549400	2.47176000	-1.06802500
O	0.24597400	-2.04149100	-1.57068200
H	1.19121700	-1.90938400	-1.38129500
H	0.02147700	-2.85204800	-1.07967300
H	-0.16591100	-2.87434600	1.28878700
H	-2.83024300	1.72246700	1.20209700
H	-3.03883200	3.89725500	0.33019900
H	-1.79393600	2.41270200	-0.97987000
O	0.54369900	0.28976900	0.81912200
O	-2.55022600	-0.79045100	-0.89779800
N	3.04364000	0.14828000	-0.29299600
N	3.99046200	-0.33016500	0.49373200
H	3.19268000	0.03556900	-1.29562700
H	2.06979100	0.20223400	0.10254500
H	3.81505100	-0.22902300	1.49351400
C	5.36600000	-0.43824300	0.02335500
H	5.87406300	-1.17743600	0.64766700
H	5.36254100	-0.79788600	-1.00962600
C	6.08431100	0.84158800	0.10077800
N	6.65431100	1.85135200	0.16582100

E = -1290.5162506 a.u.

TS1^{II}

Atom	X	Y	Z (Angstrom)
Np	-0.97523400	-0.26274700	-0.05293800
O	-0.97586700	-2.47443700	1.30429200
H	-1.42782200	-3.12043500	0.73236000
O	-2.48020300	0.92954100	1.71362500
H	-1.84359300	1.33242500	2.32945200
O	-3.15969100	2.94314900	-0.02222400
H	-4.03453100	2.90969400	-0.44675400
O	-1.00580700	1.94304400	-1.38620300
H	-0.24893700	2.45006400	-1.04390500
O	0.50385000	-2.01690800	-1.52204200
H	1.39812200	-1.79434200	-1.20377500
H	0.27308100	-2.82108300	-1.02274900
H	-0.05514300	-2.78965900	1.33984000
H	-2.81890300	1.69008700	1.17482600
H	-3.07483300	3.85354000	0.31060000
H	-1.80032100	2.38252500	-0.98421900
O	0.66192400	0.26058700	0.85832100
O	-2.53193000	-0.71706300	-0.87501900
N	2.86968100	-0.07882900	-0.27036700
N	3.92446500	-0.53501300	0.39552800
H	3.10764200	0.16989200	-1.23249500
H	1.68050000	0.08644000	0.31616900
H	3.78378100	-0.63134400	1.39865600
C	5.28702500	-0.31768400	-0.07375100
H	5.95141800	-0.99855200	0.46408200
H	5.33842500	-0.55785100	-1.14036700
C	5.74247800	1.06663700	0.13315200
N	6.09052100	2.16198600	0.30471600

E = -1290.5038334 a.u.

INT1^{II}

Atom	X	Y	Z (Angstrom)
Np	-0.94090000	-0.27079300	-0.01543500
O	-0.95966300	-2.47496600	1.34562900
H	-1.21509200	-3.18562800	0.73071700
O	-2.51227900	0.95753800	1.59957700
H	-1.93184900	1.47452100	2.18580100
O	-3.37345100	2.72931600	-0.29092800
H	-4.16903700	2.46344900	-0.78416500
O	-0.97511500	1.92938700	-1.34067600
H	-0.30834100	2.49593700	-0.91458100
O	0.65094900	-1.86826500	-1.24997600
H	1.52329600	-1.43284200	-1.05704900
H	0.65048500	-2.67730700	-0.70781200
H	-0.03497100	-2.67700600	1.57439700
H	-2.93204600	1.63112200	1.00273300
H	-3.51717700	3.66351300	-0.05986200
H	-1.84628500	2.31159000	-1.05694400
O	0.72026600	0.35896400	0.98360100
O	-2.41474000	-0.84161900	-0.90624300
N	2.92926000	-0.28125400	-0.66288400
N	4.08133300	-0.72295600	-0.15038700
H	3.14859100	0.34562300	-1.44351900
H	1.52978400	0.14597800	0.42324100
H	3.98344400	-1.21316100	0.73493700
C	5.34455400	-0.02547900	-0.36356900
H	6.16295100	-0.67453200	-0.04140200
H	5.46673500	0.17560500	-1.43271200
C	5.42123500	1.24606200	0.37584200
N	5.46236500	2.24572000	0.96757400

E = -1290.5088767 a.u.

IC2^{II}

Atom	X	Y	Z (Angstrom)
Np	-1.14289600	-0.27766100	-0.14662200
O	-1.15297100	-2.48522200	1.17827900
H	-1.14680600	-3.21697600	0.53535700
O	-3.03016800	0.09901200	1.57680000
H	-2.55670800	0.45966400	2.34672600
O	-4.00438500	2.30039500	0.26402100
H	-4.83018700	2.22611900	-0.24537300
O	-1.64969800	2.07945700	-1.09843700
H	-1.02011800	2.65251600	-0.62547300
O	0.94081400	-1.55760100	-0.97751900
H	1.78025000	-1.06741000	-0.76655700
H	0.95871100	-2.34566400	-0.40607100
H	-0.28980300	-2.54659600	1.62573300
H	-3.48432600	0.88460400	1.17361400
H	-4.10614600	3.10921800	0.79525800
H	-2.52742400	2.26112700	-0.66861200
O	0.00255900	0.52085600	1.28829700
O	-2.19930100	-1.02870600	-1.39742000
N	3.42650700	-0.23726900	-0.64072100
N	4.27367500	-0.69369300	0.28862900
H	3.92513800	-0.21959500	-1.53613800
H	0.71311000	1.13722800	0.88821600
H	3.93617600	-0.59796400	1.24286800
C	5.72137100	-0.65874600	0.11263600
H	6.18312600	-1.29911200	0.86898300
H	5.97018100	-1.05972800	-0.87504600
C	6.27516700	0.70028800	0.23532200
N	6.69304600	1.77984300	0.34074800
O	1.86819900	2.01923000	0.17416900
H	2.42312500	1.27967200	-0.18229200
H	1.42881500	2.39458700	-0.60918900

E = -1366.933740 a.u.

INT2^{II}

Atom	X	Y	Z (Angstrom)
Np	-1.31628200	-0.33478000	-0.09316500
O	-0.80126100	-2.72375500	0.83497400
H	-1.09387400	-3.32083600	0.12373900
O	-3.12221900	0.08195500	1.72116100
H	-2.60984600	0.32457300	2.51205300
O	-3.81841300	2.49904500	0.62317600
H	-4.68933900	2.55938700	0.19336400
O	-1.69632200	2.12499500	-1.08774100
H	-0.92776800	2.57796400	-0.69885700
O	0.72038200	-1.14973100	-1.64491400
H	1.46664600	-0.83196900	-1.10786300
H	0.66809000	-2.09958600	-1.43458000
H	0.16862000	-2.80907800	0.83366300
H	-3.47565400	0.94754600	1.38738100
H	-3.78697700	3.25629700	1.23373600
H	-2.45772100	2.38112500	-0.50799300
O	-0.02993300	0.40537200	1.00402300
O	-2.59030700	-1.06666800	-1.17234900
N	3.94539100	0.52934500	-0.48275200
N	4.55272100	0.28733700	0.66551100
H	4.04787600	-0.19141100	-1.19744300
H	1.05047000	1.46286400	0.07666900
H	4.43374900	1.00496900	1.38014400
C	5.72379000	-0.57814000	0.72334200
H	5.84420700	-0.90544700	1.75887900
H	5.54740600	-1.45927500	0.09835300
C	6.94836700	0.10428000	0.28152400
N	7.91826800	0.64134400	-0.06428500
O	1.69170300	2.04171400	-0.41049500
H	3.08076100	1.14374400	-0.45894500
H	1.37094300	2.02727000	-1.32916900

E = -1366.938352 a.u.

$IC3^{II}$

Atom	X	Y	Z (Angstrom)
Np	1.11698500	-0.31888700	0.03965400
O	1.87110500	-2.41264400	-1.19669100
H	1.71141900	-2.31087600	-2.15236600
O	2.30382600	1.23142500	-1.57853600
H	1.68921700	1.31265700	-2.32961800
O	2.04292300	3.50648400	-0.21042600
H	1.42715500	3.08818800	0.42957900
O	0.35047700	1.79082500	1.29193200
H	-0.61479800	1.89248600	1.20203300
O	-0.36697300	-1.43636500	1.79630600
H	-0.99427900	-2.02477100	1.33847600
H	0.18076500	-2.02809100	2.34337500
H	2.83865700	-2.48678800	-1.10860800
H	2.26646700	2.12601100	-1.11730200
H	2.87520200	3.59357900	0.28583800
H	0.51796100	1.72195500	2.24960100
O	-0.30297400	-0.25498400	-0.99557200
O	2.52566700	-0.38478700	1.07047400
H	-2.07590300	-0.12985900	-0.23311800
N	-3.01069600	-0.00016000	0.17062300
N	-3.84603400	0.78092400	-0.48787600
H	-3.67059300	0.86678400	-1.48952300
C	-5.18285400	1.04056400	0.03260200
H	-3.14349200	-0.07927400	1.17873600
H	-5.55631500	1.94263400	-0.45795400
H	-5.11472200	1.22851900	1.10858200
C	-6.10637300	-0.07265100	-0.22341800
N	-6.83946500	-0.94988000	-0.42710700

E = -1290.3250776 a.u.

TS3^{II}

Atom	X	Y	Z (Angstrom)
Np	1.08156800	-0.30285300	0.04325900
O	1.86710000	-2.40702400	-1.19922000
H	1.70872900	-2.29549800	-2.15356800
O	2.27908100	1.23753000	-1.59607700
H	1.69639800	1.25635000	-2.37594000
O	1.87223900	3.54201900	-0.29660200
H	1.29296400	3.10838800	0.36754400
O	0.28831300	1.82200700	1.29795400
H	-0.67692200	1.93389900	1.22491300
O	-0.42844200	-1.45432300	1.79909400
H	-0.73177600	-2.29409400	1.40916000
H	0.12547800	-1.71889000	2.55568400
H	2.83499900	-2.47048700	-1.11234000
H	2.17138100	2.14292700	-1.17348000
H	2.70788400	3.68977800	0.17879100
H	0.47096600	1.77828900	2.25389000
O	-0.46901400	-0.26884300	-1.00698800
O	2.54437100	-0.34985900	1.04594200
H	-1.55012200	-0.25027400	-0.41931800
N	-2.64607000	-0.14808000	0.18153200
N	-3.64450600	0.38430800	-0.38944400
H	-3.55417600	0.55131700	-1.39891000
C	-4.88315600	0.79842800	0.28126700
H	-2.74999600	-0.29946100	1.19287000
H	-5.00378500	1.87550100	0.11203000
H	-4.78916900	0.60579500	1.35263600
C	-6.03053400	0.08071900	-0.27555300
N	-6.95024600	-0.47839600	-0.70982200

E = -1290.2880103 a.u.

INT3^{II}

Atom	X	Y	Z (Angstrom)
Np	1.23520700	-0.23938900	-0.00117700
O	2.78966500	-1.95782400	-1.11397400
H	2.66866600	-1.89688200	-2.07851900
O	2.05253700	1.80734500	-1.32298300
H	1.54352400	1.79384000	-2.15235700
O	1.00304400	3.80704000	0.12386700
H	0.45374300	3.14819900	0.60669900
O	-0.26836600	1.56482400	1.20591800
H	-1.22733800	1.49819700	1.05283200
O	0.07653200	-1.98517900	1.53203900
H	0.05050900	-2.81727400	1.02608600
H	0.70103400	-2.16235400	2.25821200
H	3.71865600	-1.70739300	-0.96468500
H	1.71372500	2.61079200	-0.82807200
H	1.70123100	4.04050800	0.75947200
H	-0.15869900	1.50558400	2.17213800
O	-0.19315800	-0.53985100	-1.42263800
O	2.52799400	0.01670800	1.23488200
H	-1.08589100	-0.60569400	-1.01492600
N	-3.03302500	-0.69063400	0.13180100
N	-4.02061400	-0.02502600	-0.16117700
H	-3.95225300	0.53196400	-1.02994300
C	-5.28237900	0.10708700	0.61188300
H	-3.18759100	-1.21583000	1.01226900
H	-5.24821300	1.09857400	1.08224400
H	-5.30982400	-0.66719700	1.38324300
C	-6.43115500	0.01867200	-0.28257600
N	-7.35782900	-0.04875200	-0.97747700

E = -1290.3263432 a.u.

INT4^{II}

Atom	X	Y	Z (Angstrom)
Np	-1.18275700	-0.51585700	-0.09970600
O	-2.42728400	-2.63435100	0.63418400
H	-3.08583000	-2.39650300	1.31081200
O	-3.30656400	0.72130900	-0.84200500
H	-3.83482300	0.72053400	-0.02313400
O	-2.16803500	3.15554200	-0.64923100
H	-1.25195200	2.81720600	-0.78882300
O	0.07444700	1.59814500	-0.91061200
H	0.95865100	1.76215200	-0.51093600
O	1.49876000	-1.25527000	0.67334200
H	1.70682800	-0.44410800	1.17259200
H	1.36167600	-1.92961500	1.36418500
H	-2.94771300	-2.98357100	-0.11106400
H	-2.97887200	1.66156100	-0.90514700
H	-2.28600200	3.90432100	-1.25733100
H	0.24631700	1.46950800	-1.86079200
O	-1.43113000	0.17394700	1.75845800
O	-0.97951600	-1.17957300	-1.75472000
H	-1.97243200	1.03971800	1.81418100
N	6.57635900	-0.33932700	0.91849400
N	5.61560000	-0.02457300	0.22066300
C	5.35411600	1.34255600	-0.29399300
H	5.64425500	1.34598200	-1.35231300
H	5.95696900	2.07382300	0.25192200
C	3.93047200	1.64356100	-0.18210500
N	2.80053400	1.88041300	-0.09751700
H	7.16828900	0.48526000	1.13021300
H	4.88284100	-0.84096600	-0.07353300
O	3.95044300	-1.87239000	-0.44180500
H	3.06812500	-1.65485800	-0.03763900
H	3.81123100	-1.78425000	-1.40230900
O	-2.80621300	2.43938100	1.93261800
H	-3.73960000	2.17411900	1.85883200
H	-2.60578900	2.84813800	1.05623500

E = -1443.206118 a.u.

INT5^{II}

Atom	X	Y	Z (Angstrom)
Np	-1.21502500	-0.51565800	-0.11494400
O	-2.46972700	-2.63901200	0.62347700
H	-3.12064400	-2.39525400	1.30511200
O	-3.33766400	0.72766300	-0.85714600
H	-3.87897200	0.72106500	-0.04707300
O	-2.18886800	3.16296400	-0.63650200
H	-1.27164100	2.82584900	-0.77134800
O	0.05155200	1.60535600	-0.92125700
H	0.93837700	1.72452800	-0.51196600
O	1.74501200	-1.23253400	0.76816800
H	1.84129700	-0.27091300	0.90905400
H	1.68287600	-1.60943000	1.66573600
H	-3.00257500	-2.97288600	-0.12000300
H	-3.00697000	1.66691600	-0.90763200
H	-2.30210400	3.91587500	-1.24035200
H	0.22268600	1.50271900	-1.87450200
O	-1.51293600	0.18729100	1.73741800
O	-0.85925600	-1.23654100	-1.72993800
H	-2.05491000	1.05444700	1.79885800
N	6.82222700	-0.10434200	0.71727800
N	5.73705400	0.03681700	0.14782300
C	5.33701100	1.39030800	-0.33323900
H	5.55725100	1.42924700	-1.40728000
H	5.89488300	2.18444900	0.17552300
C	3.90200700	1.57433200	-0.14387100
N	2.76075700	1.70364400	0.01044100
H	7.33172900	0.79779600	0.81845400
H	4.67906100	-1.23958900	-0.07819000
O	3.99042300	-2.00107400	-0.18999800
H	3.07360500	-1.67997100	0.20185700
H	3.86600300	-2.14088700	-1.15225000
O	-2.87597700	2.44589600	1.92688400
H	-3.80869300	2.18346500	1.83521000
H	-2.65880400	2.85799900	1.05561300

E = -1443.221738 a.u.

INT6^{II}

Atom	X	Y	Z (Angstrom)
Np	1.03520500	-0.50977100	-0.12209400
O	2.29828400	-2.63824600	-0.91075800
H	3.10644700	-2.38585200	-1.39032200
O	3.15756900	0.25369000	1.16398400
H	3.87419300	0.16751100	0.51071200
O	2.54102200	2.97742500	1.11066000
H	1.58385200	2.73442800	1.21833300
O	0.22180900	1.62837700	1.16178800
H	-0.64296600	1.90894800	0.78269100
O	-1.93561200	-2.39189800	0.13921200
H	-2.00746500	-3.36150500	0.21375700
H	-1.12470200	-2.14875900	0.65713800
H	2.61847400	-3.09784100	-0.11502700
H	3.08082400	1.22389800	1.30773300
H	2.66858500	3.85565500	1.51069600
H	0.02095700	1.34734200	2.07230900
O	1.62419200	0.45249400	-1.61832200
O	0.42930500	-1.48709700	1.32266700
H	2.35276800	1.77735100	-1.49975300
N	-6.19090900	-0.12158800	-1.05049400
N	-5.27495600	0.28897000	-0.33251300
C	-4.95660800	1.74681000	-0.32902700
H	-5.51879900	2.19720200	0.49826300
H	-5.25444300	2.23102800	-1.26687300
C	-3.53119700	1.94331100	-0.08716800
N	-2.39853600	2.08985200	0.10905900
H	-6.62295200	0.64055900	-1.61270100
H	-4.40431400	-0.78752500	0.67071700
O	-3.91456300	-1.43331500	1.29322200
H	-3.04302800	-1.84230100	0.78347100
H	-3.59005500	-0.90037000	2.04764800
O	2.83679000	2.69517600	-1.37688700
H	3.78741900	2.54068600	-1.55539400
H	2.74844600	2.91404300	-0.34834800

E = -1443.215449 a.u.

Cartesian coordinates and energies of Pathway III

$IC1^{III}$

Atom	X	Y	Z (Angstrom)
Np	-0.94846800	0.01402500	0.12161500
O	-1.76296500	2.91785400	-0.97259300
H	-1.64653300	2.27412700	-1.69351600
O	-2.76668200	-0.40892100	-1.68945600
H	-2.37324400	-1.03259400	-2.32538900
O	-1.35134200	-2.67594800	0.12251700
H	-1.84241500	-2.77420400	0.95727900
O	0.61218900	-1.09495200	1.93112900
H	1.00635000	-1.87093800	1.49621200
O	0.46598600	2.39485100	0.60185800
H	-0.24973900	2.77065500	0.02985000
H	0.17704700	2.61022000	1.50512000
H	-2.39737300	2.47301300	-0.38227400
H	-3.47781400	-0.91914200	-1.26196000
H	-2.04505300	-2.71267700	-0.56002900
H	1.35250800	-0.46711700	2.01308000
O	0.34926700	-0.27717200	-1.18325400
O	-2.23656000	0.31298800	1.39121800
N	2.63341400	-1.80072400	-0.92960300
N	3.76416800	-1.18831400	-0.62813300
H	1.75926800	-1.22398300	-0.99977600
H	2.73192400	-2.66589600	-1.45758800
H	4.59508700	-1.77999700	-0.59460200
C	3.71891400	0.00894200	0.20755700
H	2.83278800	0.59278400	-0.05795800
H	3.65045600	-0.26905800	1.26752200
C	4.91767100	0.81826700	-0.00923900
N	5.86465300	1.47156400	-0.16331900

E = -1290.5101527 a.u.

TS1^{III}

Atom	X	Y	Z (Angstrom)
Np	-0.928483	0.012234	0.131135
O	-1.756315	2.938219	-0.888730
H	-1.641420	2.313902	-1.626159
O	-2.748867	-0.373141	-1.670946
H	-2.369001	-0.982127	-2.329264
O	-1.371005	-2.601929	-0.014382
H	-1.832035	-2.805793	0.818559
O	0.675948	-1.201344	1.751903
H	1.297534	-1.617813	1.119398
O	0.482907	2.383288	0.647354
H	-0.247854	2.775329	0.106257
H	0.222374	2.571557	1.565309
H	-2.405659	2.487079	-0.320545
H	-3.473823	-0.878403	-1.261514
H	-2.061041	-2.696001	-0.694632
H	1.200772	-0.488139	2.160196
O	0.421699	-0.272060	-1.243638
O	-2.207207	0.289089	1.401714
N	2.394609	-1.718851	-0.715983
N	3.604884	-1.192515	-0.551596
H	1.351297	-0.938935	-0.978551
H	2.469680	-2.635890	-1.158734
H	4.402754	-1.827610	-0.554848
C	3.712734	0.012346	0.263639
H	2.833542	0.637359	0.087334
H	3.748647	-0.237924	1.332149
C	4.916620	0.766171	-0.091021
N	5.871900	1.371018	-0.355627

E = -1290.4974135 a.u.

INT1^{III}

Atom	X	Y	Z (Angstrom)
Np	0.94661900	-0.00533300	-0.09553100
O	1.95201800	3.00657500	0.55037400
H	1.92552900	2.41302500	1.32144200
O	2.76438700	-0.37494600	1.70594200
H	2.38078100	-0.96690100	2.37781000
O	1.35845800	-2.58764100	0.10914600
H	1.79191600	-2.84250100	-0.72484500
O	-0.66883500	-1.20269700	-1.69391800
H	-1.39513900	-1.45082300	-1.06221300
O	-0.46240800	2.33652700	-0.62785000
H	0.33294800	2.76648300	-0.22214300
H	-0.31084300	2.41684800	-1.58559400
H	2.48697600	2.50623300	-0.09191600
H	3.49105100	-0.88950400	1.31123400
H	2.05309700	-2.70014700	0.78194000
H	-1.05137400	-0.49027600	-2.23822100
O	-0.44402800	-0.31338900	1.33299000
O	2.22045700	0.26436900	-1.36273500
N	-2.57391300	-1.79337300	0.33453200
N	-3.77466000	-1.20735900	0.32409300
H	-1.22115900	-0.86513400	0.98465100
H	-2.70292600	-2.75489900	0.65771200
H	-4.60899400	-1.79312800	0.33060900
C	-3.87795300	0.07551100	-0.35660000
H	-2.92711700	0.60388700	-0.24395000
H	-4.07503600	-0.04947400	-1.42978800
C	-4.94643500	0.89000400	0.22855200
N	-5.79704500	1.53913700	0.68056600

E = -1290.5007048 a.u.

$IC2^{III}$

Atom	X	Y	Z (Angstrom)
Np	-1.39016200	-0.32760900	0.04438500
O	-2.48773500	3.40690100	-0.67782800
H	-2.84323300	2.57559200	-1.06703600
O	-3.19804900	0.82515700	-1.47707800
H	-3.07593800	0.62928500	-2.42357300
O	-1.05041700	-2.88767800	-0.30611200
H	-1.88404700	-3.34124500	-0.08850100
O	0.42530800	-0.73041400	1.82648400
H	1.21571100	-0.43785500	1.29454400
O	-0.87009900	2.02459600	0.98002100
H	-1.44316300	2.60947200	0.40156400
H	-1.30097400	2.04047000	1.85237000
H	-3.20183700	3.71286000	-0.09253900
H	-4.11111200	0.55444700	-1.27375800
H	-0.92648600	-3.04567500	-1.25873500
H	0.27782600	-0.01374500	2.46913400
O	0.02214500	-0.02556000	-1.35494200
O	-2.69468300	-0.59261400	1.27364500
N	4.57133100	-1.39750400	-0.38764600
N	5.81829900	-0.90732600	-0.36836000
H	0.93603900	0.03633200	-0.92400600
H	4.64333700	-2.40611500	-0.23338400
H	6.60087400	-1.53165400	-0.54974100
C	6.00710900	0.47193800	-0.78653000
H	7.07929900	0.66098500	-0.88215000
H	5.53685200	0.66862100	-1.75865000
C	5.45014800	1.41575100	0.19442100
N	5.00119400	2.16567700	0.96030800
O	2.29933300	0.08727100	0.04285400
H	2.60690000	0.99370100	0.21531700
H	3.12928100	-0.45116600	-0.14251300

E = -1366.945118 a.u.

TS2^{III}

Atom	X	Y	Z (Angstrom)
Np	-1.34281600	-0.31326900	0.08168900
O	-2.02377600	3.38846400	-1.04149100
H	-2.53115800	2.58189500	-1.28815200
O	-3.10858900	0.84217900	-1.46308400
H	-3.01394300	0.58372000	-2.39759000
O	-1.02558900	-2.87201100	-0.27072000
H	-1.85669000	-3.33375900	-0.06207100
O	0.46200000	-0.71922700	1.88942400
H	1.22729500	-0.34059300	1.40211000
O	-0.85784400	2.06082200	1.00944100
H	-1.24144800	2.62409000	0.27577300
H	-1.48570500	2.16444400	1.74558700
H	-2.68061600	3.95284400	-0.59877500
H	-4.03580900	0.65058000	-1.23619000
H	-0.88729400	-3.03106100	-1.22098500
H	0.26312500	-0.06917200	2.58615000
O	0.01801700	-0.02944000	-1.23137000
O	-2.63609500	-0.58236000	1.32646400
N	4.09127000	-1.21415100	-0.97140200
N	5.37413400	-0.89684700	-0.79456000
H	1.16919600	0.13491500	-0.70101000
H	4.01862500	-2.21680900	-1.14909100
H	6.09092400	-1.53777900	-1.12442200
C	5.74054000	0.50629100	-0.69921700
H	6.82388000	0.58521000	-0.81682300
H	5.26636800	1.09321500	-1.49503800
C	5.36448300	1.08917500	0.59882000
N	5.06301200	1.56011800	1.61727100
O	2.17152600	0.25401400	-0.11863700
H	2.45214700	1.18832200	-0.16167300
H	2.97677300	-0.35224400	-0.51191700

E = -1366.925780 a.u.

INT2^{III}

Atom	X	Y	Z (Angstrom)
Np	-1.39278700	-0.32480400	0.05883200
O	-2.40895500	3.45856000	-0.88000400
H	-2.79579000	2.60892000	-1.19523400
O	-3.21812300	0.85918300	-1.47240600
H	-3.12012100	0.63928600	-2.41597000
O	-1.04365300	-2.90408600	-0.32216900
H	-1.88673000	-3.35135300	-0.13182900
O	0.41209500	-0.73827500	1.88818800
H	1.22010500	-0.45232500	1.39337300
O	-1.00366800	2.13294900	1.03334700
H	-1.48891100	2.68833000	0.36059000
H	-1.58924300	2.12813000	1.80945600
H	-3.12984200	3.86662100	-0.37044500
H	-4.14428200	0.65023100	-1.25808500
H	-0.90866900	-3.03890500	-1.27631900
H	0.24295700	-0.02274600	2.52566300
O	-0.08491400	-0.05356500	-1.23476900
O	-2.69428900	-0.59108800	1.32506800
N	4.61573700	-1.44270500	-0.49915200
N	5.61451800	-0.72256000	-0.97094500
H	1.56320200	0.00666300	-0.53190100
H	4.74520100	-2.45150900	-0.48138100
H	6.52738700	-1.17495200	-1.00091600
C	5.53203900	0.73165300	-0.94780500
H	6.34811400	1.11785700	-1.56189100
H	4.58157100	1.04136400	-1.39236500
C	5.63574400	1.28227100	0.41202800
N	5.71107900	1.72068500	1.48484900
O	2.34586400	-0.03101900	0.07884800
H	2.64245500	0.89098600	0.18120100
H	3.69092300	-0.97258300	-0.34275100

E = -1366.954722 a.u.

$IC3^{III}$

Atom	X	Y	Z (Angstrom)
Np	-0.87891700	-0.11621600	0.05573700
O	-2.21057200	-0.11634300	-2.14972300
H	-2.92466300	-0.76102500	-1.99419500
O	-0.29929600	-2.41633400	-0.90077500
H	0.66957200	-2.50044500	-0.83687200
O	0.57027000	-1.17593100	1.87885600
H	1.41100100	-1.47409800	1.47089400
O	-0.48763300	1.71272500	1.83714100
H	0.39145200	2.07519400	1.62404300
O	-2.27739500	2.28255900	-0.30448000
H	-2.00235500	2.76596700	-1.10302400
H	-3.24376800	2.19904100	-0.38020000
H	-2.64622100	0.75151100	-2.05393000
H	-0.64631900	-3.06710700	-0.26377700
H	0.81657900	-0.41641100	2.43860700
H	-1.11664300	2.34394300	1.42805600
O	0.50317600	0.56707900	-0.79293500
O	-2.25031100	-0.81518800	0.88659000
H	2.29661600	1.43130900	-0.57496400
H	3.12162800	2.85249600	0.08349600
N	3.16202600	1.94816700	-0.38378100
N	4.28499300	1.27008700	-0.25276600
H	5.10521800	1.79970100	0.03812300
C	4.44228200	-0.05924100	-0.82692600
H	5.50648600	-0.30278400	-0.80308300
H	4.10194300	-0.06669400	-1.86836300
C	3.69219100	-1.06390900	-0.06308400
N	3.08241600	-1.84570500	0.53858900

E = -1290.3207694 a.u.

TS3^{III}

Atom	X	Y	Z (Angstrom)
Np	-0.81643700	-0.13393200	0.06529300
O	-2.15165300	-0.15344400	-2.13886100
H	-2.85067700	-0.81880900	-2.00281900
O	-0.28853900	-2.48729700	-0.86458200
H	0.68412900	-2.54664000	-0.88682700
O	0.67763800	-1.30596900	1.81237400
H	1.54553900	-1.52591200	1.41822900
O	-0.44611400	1.69835800	1.84833800
H	0.43351700	2.10657800	1.76543500
O	-2.21900300	2.27078600	-0.30851900
H	-1.98081000	2.74007500	-1.12704100
H	-3.18400100	2.15658100	-0.35747400
H	-2.61108000	0.70141900	-2.04217700
H	-0.55228500	-3.10678100	-0.16018400
H	0.87323100	-0.63763700	2.49341300
H	-1.05586600	2.33584600	1.42084400
O	0.66668800	0.46939000	-0.92102100
O	-2.24229100	-0.71585100	0.94030500
H	1.57052300	1.14279600	-0.56504500
H	2.49994300	2.78233100	0.25490600
N	2.59336600	1.88068100	-0.22561300
N	3.80285400	1.48075600	-0.29039100
H	4.54866200	2.05916500	0.11014800
C	4.16002700	0.21028600	-0.92812200
H	5.24715800	0.18303500	-1.02317500
H	3.70856500	0.17045800	-1.92515300
C	3.69582200	-0.92789500	-0.12867900
N	3.30995200	-1.81700500	0.50902900

E = -1290.2849527 a.u.

INT3^{III}

Atom	X	Y	Z (Angstrom)
Np	-1.03073000	-0.05837300	0.02539700
O	-2.38448300	-0.07541200	-2.18295800
H	-3.24843000	-0.46506600	-1.95947600
O	-0.46055200	-2.62771900	-0.43077800
H	0.51305500	-2.66252900	-0.41614900
O	0.40067400	-1.04738900	1.93942800
H	1.19333400	-1.41774500	1.50270000
O	-0.61759900	1.74619500	1.84769200
H	0.32798500	1.97067000	1.78571500
O	-2.06367100	2.43078700	-0.37546600
H	-1.70944800	2.72299200	-1.23364600
H	-3.01796300	2.31440000	-0.52847500
H	-2.58703300	0.85384500	-2.39221800
H	-0.72564200	-3.08419200	0.38707500
H	0.73549500	-0.31152700	2.48207800
H	-1.07273200	2.44313700	1.33166000
O	0.63729600	0.59156100	-0.99908300
O	-2.52431700	-0.60878900	0.88868300
H	0.97854600	1.39438400	-0.54802500
H	5.62158000	2.36488300	0.54891600
N	5.12403700	1.87137400	-0.21349300
N	5.13449300	0.66507700	0.01240500
H	5.58600100	0.26378700	0.85589900
C	4.52931200	-0.28815900	-0.94088100
H	5.34834400	-0.89113800	-1.35206900
H	4.04571200	0.28515600	-1.73437400
C	3.56947200	-1.14717800	-0.25202100
N	2.79540600	-1.82420300	0.28190500

E = -1290.3182662 a.u.

INT4^{III}

Atom	X	Y	Z (Angstrom)
Np	0.97792900	0.34045700	-0.15624000
O	3.08596200	-1.40999000	-0.18343100
H	3.26546300	-1.62030900	-1.11604300
O	0.21277600	-1.80723000	-1.38155900
H	0.48161300	-2.47581200	-0.71175900
O	-1.50639900	1.34744700	-0.58887300
H	-1.32729900	1.86088300	-1.39925700
O	2.60855100	1.56380700	1.40311300
H	2.41963900	1.23020300	2.29733500
O	4.95643200	0.35789500	0.69796300
H	5.58469600	0.12168100	1.40215900
H	5.49461900	0.78166000	0.00701300
H	3.85967200	-0.86791800	0.11968300
H	-0.76443600	-1.78260100	-1.31347600
H	-1.88240800	0.50833600	-0.92076300
H	3.51565700	1.22059500	1.19221100
O	0.35255900	-0.63042200	1.49905100
O	1.54456200	1.24769300	-1.61215500
H	0.62767700	-1.59993100	1.43893500
H	-6.07532200	1.04163300	1.99243400
N	-6.09169200	0.09382900	1.57589700
N	-5.33212300	0.09339500	0.60725000
H	-4.74191000	1.03457200	0.29922500
C	-5.22718900	-1.14402400	-0.19084800
H	-5.83809100	-1.00012900	-1.09117400
H	-5.61952800	-1.98397900	0.38771900
C	-3.84031200	-1.37983400	-0.58594800
N	-2.74575400	-1.57305500	-0.91329000
O	-4.06443300	2.24562600	0.04791200
H	-3.11633200	2.00539000	-0.11617900
H	-4.39164500	2.57007200	-0.81152100
O	1.25804400	-3.08570000	0.91968400
H	1.43586900	-3.79136400	1.56390800
H	2.13218200	-2.70455200	0.66797800

E = -1443.221288 a.u.

INT5^{III}

Atom	X	Y	Z (Angstrom)
Np	-0.88755500	-0.20145200	-0.15746100
O	-3.08311900	1.16747000	-0.13385300
H	-3.24511700	1.47272400	-1.04387700
O	-0.34203900	2.16332200	-1.07514100
H	-0.60117000	2.71639800	-0.30696000
O	1.47662000	-1.68368900	-0.63916800
H	1.10327100	-2.52278300	-0.97002500
O	-2.40481700	-1.93330200	0.98950000
H	-2.28474100	-1.80424600	1.94657500
O	-4.83914500	-0.81366700	0.42181300
H	-5.50127900	-0.67603700	1.12142400
H	-5.34115500	-1.13160300	-0.34872600
H	-3.81312800	0.52087800	0.06615200
H	0.63773900	2.11446300	-1.02876500
H	1.78934900	-1.22349000	-1.44156200
H	-3.33652200	-1.64368500	0.81254300
O	-0.39690700	0.55778700	1.64996000
O	-1.29314100	-0.91866600	-1.76230900
H	-0.77761600	1.49082300	1.71502600
H	6.25839100	-0.65858200	1.91172600
N	6.19745100	0.12462400	1.23896200
N	5.24120800	-0.10852000	0.48894900
H	4.26066400	-1.42450400	0.56319300
C	5.06431700	0.91298900	-0.57017200
H	5.41011800	0.46651900	-1.51044000
H	5.65854700	1.80618300	-0.35445300
C	3.65379500	1.26856400	-0.71622200
N	2.54394300	1.57781000	-0.84562300
O	3.63158700	-2.24783800	0.64670600
H	2.75260000	-2.02720100	0.14132600
H	4.05796700	-2.98780900	0.16503600
O	-1.55533300	2.95467600	1.36110600
H	-1.86877200	3.51289600	2.09278500
H	-2.35306400	2.51863700	0.98633300

E = -1443.224317 a.u.

INT6^{III}

Atom	X	Y	Z (Angstrom)
Np	-0.92578000	-0.57648700	-0.10636300
O	-3.14991900	2.62589400	-0.39488200
H	-3.63685800	3.46991300	-0.41637500
O	-0.13339500	1.52235600	-1.43082600
H	-0.15905900	2.26210200	-0.79927000
O	1.86704200	-1.71909200	-0.42668000
H	1.93119200	-2.56524300	-0.90729500
O	-3.05355800	-1.32804200	1.16406400
H	-2.90563200	-1.06635000	2.08900400
O	-4.79073400	0.57835000	0.20489300
H	-5.47256600	0.82304900	0.85597800
H	-5.28989000	0.27912600	-0.57626000
H	-3.82930200	1.92257500	-0.18562400
H	0.82397900	1.36961300	-1.58297700
H	2.08735100	-1.03286700	-1.08683400
H	-3.74721700	-0.69902100	0.83773500
O	-0.39747700	0.31574900	1.44822900
O	-1.45705000	-1.43333100	-1.62811100
H	-1.08140800	1.76205700	1.46620900
H	6.11734900	0.64266400	2.24900200
N	6.12707600	1.08827600	1.31564000
N	5.31871200	0.47383900	0.60836600
H	4.33820100	-0.81104300	1.05849900
C	5.25887200	0.97864400	-0.78508300
H	5.80873200	0.26826200	-1.41453700
H	5.71811900	1.96818300	-0.87055400
C	3.86948800	1.01970900	-1.23503700
N	2.76316600	1.04915400	-1.58143700
O	3.69587800	-1.56674400	1.34206700
H	2.95512200	-1.65653100	0.60410400
H	4.20667300	-2.40305100	1.34996400
O	-1.54100700	2.67958700	1.46838500
H	-2.02598800	2.74397300	2.31559300
H	-2.29229400	2.66902800	0.65102500

E = -1443.221213 a.u.