Electronic supplementary information

Size-dependent reactivity of Rh cationic clusters to reduce NO by CO in gas phase at high temperatures

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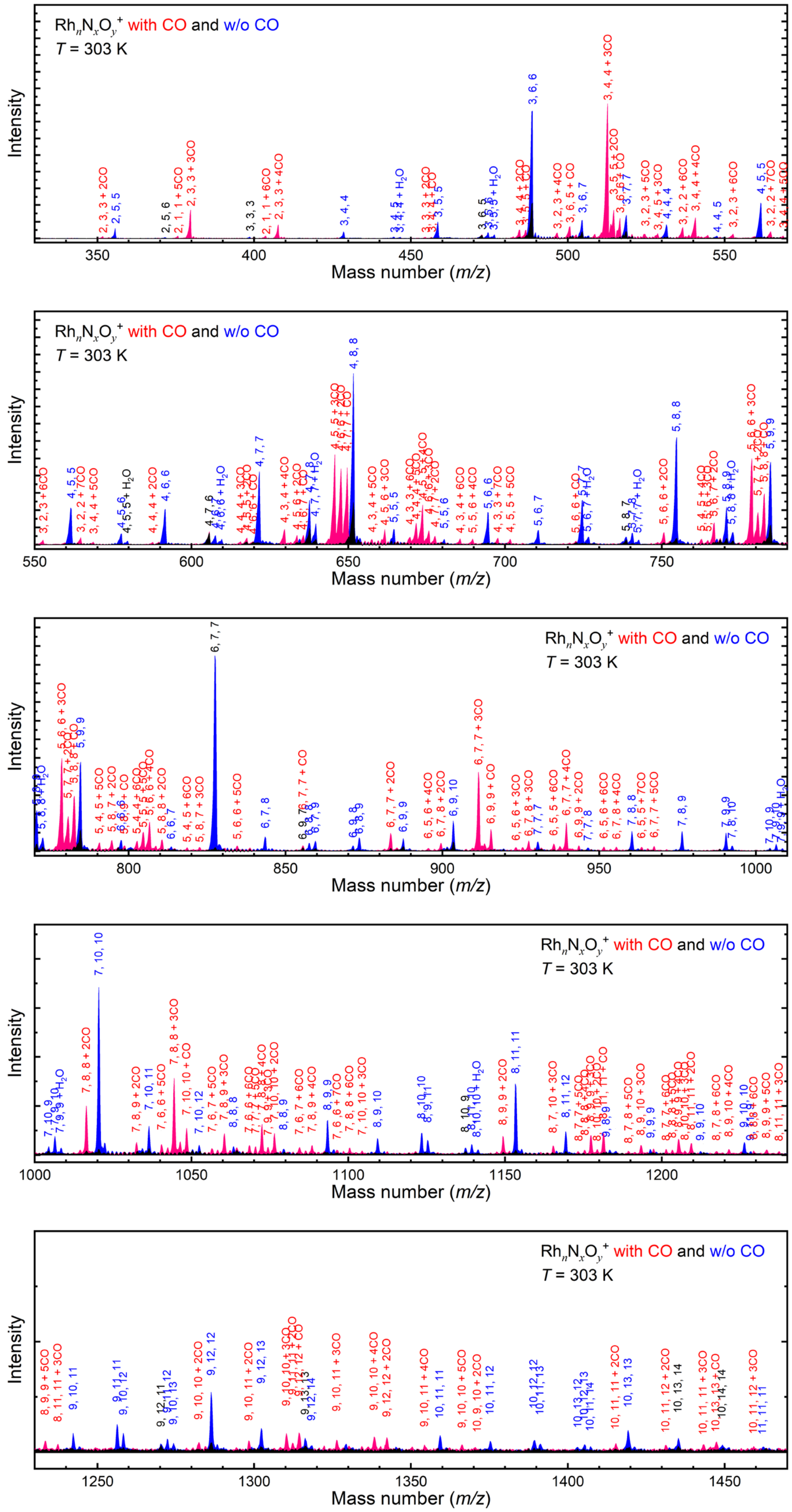

$Rh_nN_xO_y^+$ with CO and w/o CO
T = 303 K
Intensity
Mass number (m/z)
350 400 450 500 550
550 600 650 700 750
800 850 900 950 1000
1000 1050 1100 1150 1200
1250 1300 1350 1400 1450

Fig. S1 Mass spectra of $Rh_{2-10}N_xO_y^+$ cluster ions measured using an extension tube in an unheated state with and without CO gas injection. The entire mass spectrum was divided into four sections to clearly display peak assignments. The color of the peak fills in the mass spectrum corresponds to blue for no reaction with CO, red for reaction with CO, and black for the common areas. Each mass peak is attributed to the composition $Rh_nN_xO_y^+$ of the cluster in the simplified form n, x, y. The CO adduct is denoted as $Rh_nN_xO_y(CO)_k^+$ in the form n, x, y + kCO. The colors on the label indicate blue for a decrease in the response to CO, red for an increase, and black for a small change.

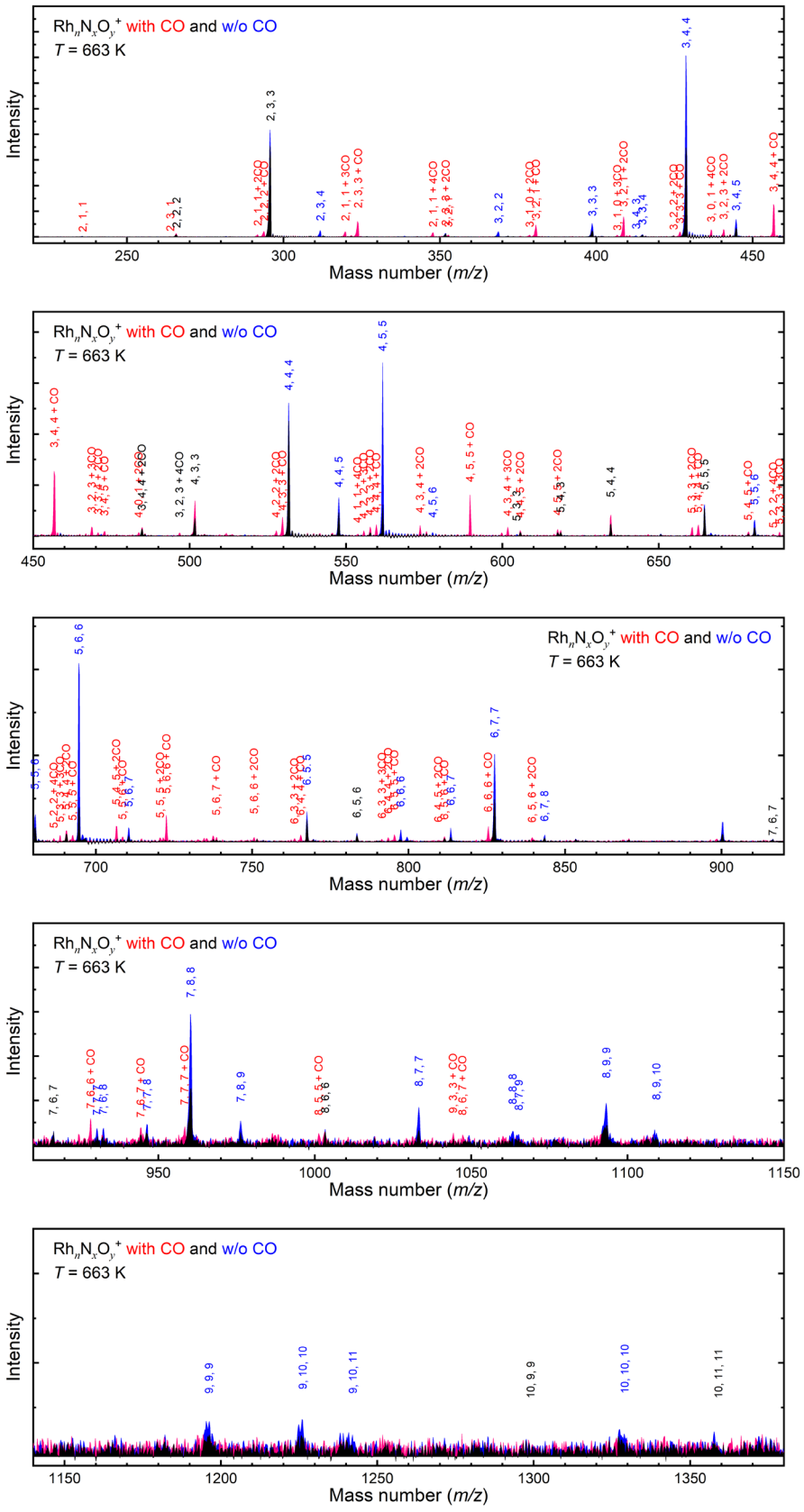

Rh$_n$N$_x$O$_y^+$ with CO and w/o CO
T = 663 K
Intensity
Mass number (m/z)

Fig. S2 Mass spectra of $Rh_{2–10}N_xO_y^+$ cluster ions after heating in an extension tube at 663 K with and without CO gas injection. The entire mass spectrum was divided into four sections to clearly display peak assignments. The color of the peak fills in the mass spectrum corresponds to blue for no reaction with CO, red for reaction with CO, and black for the common areas. Each mass peak is attributed to the composition $Rh_nN_xO_y^+$ of the cluster in the simplified form *n*, *x*, *y*. The colors on the label indicate blue for a decrease in the response to CO, red for an increase, and black for a small change.

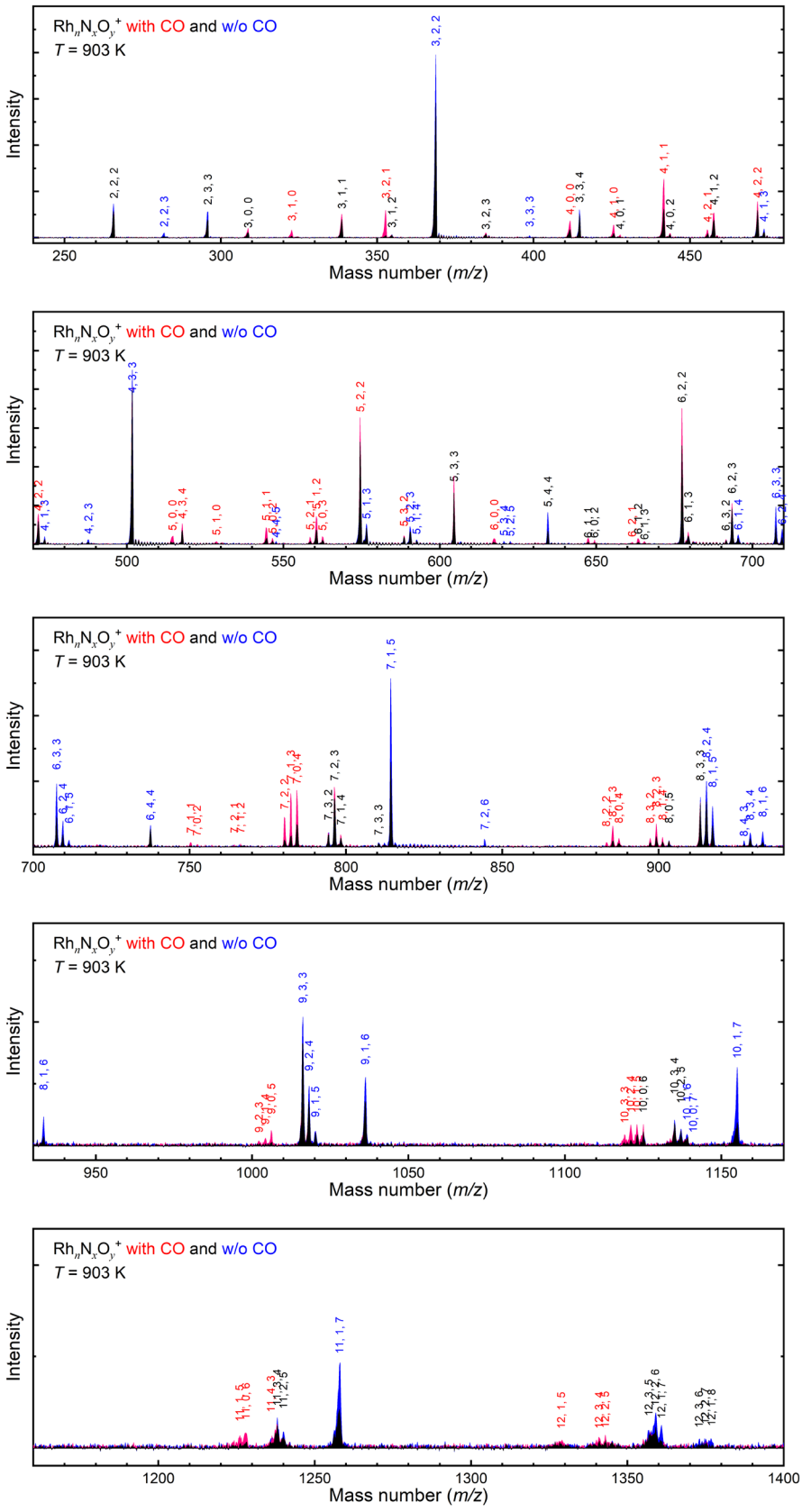

Rh$_n$N$_x$O$_y^+$ with CO and w/o CO
T = 903 K
Intensity
Mass number (m/z)

Fig. S3 Mass spectra of $Rh_{2–12}N_xO_y^+$ cluster ions after heating in an extension tube at 903 K with and without CO gas injection. The entire mass spectrum was divided into four sections to clearly display peak assignments. The color of the peak fills in the mass spectrum corresponds to blue for no reaction with CO, red for reaction with CO, and black for the common areas. Each mass peak is attributed to the composition $Rh_nN_xO_y^+$ of the cluster in the simplified form *n*, *x*, *y*. The colors on the label indicate blue for a decrease in the response to CO, red for an increase, and black for a small change.

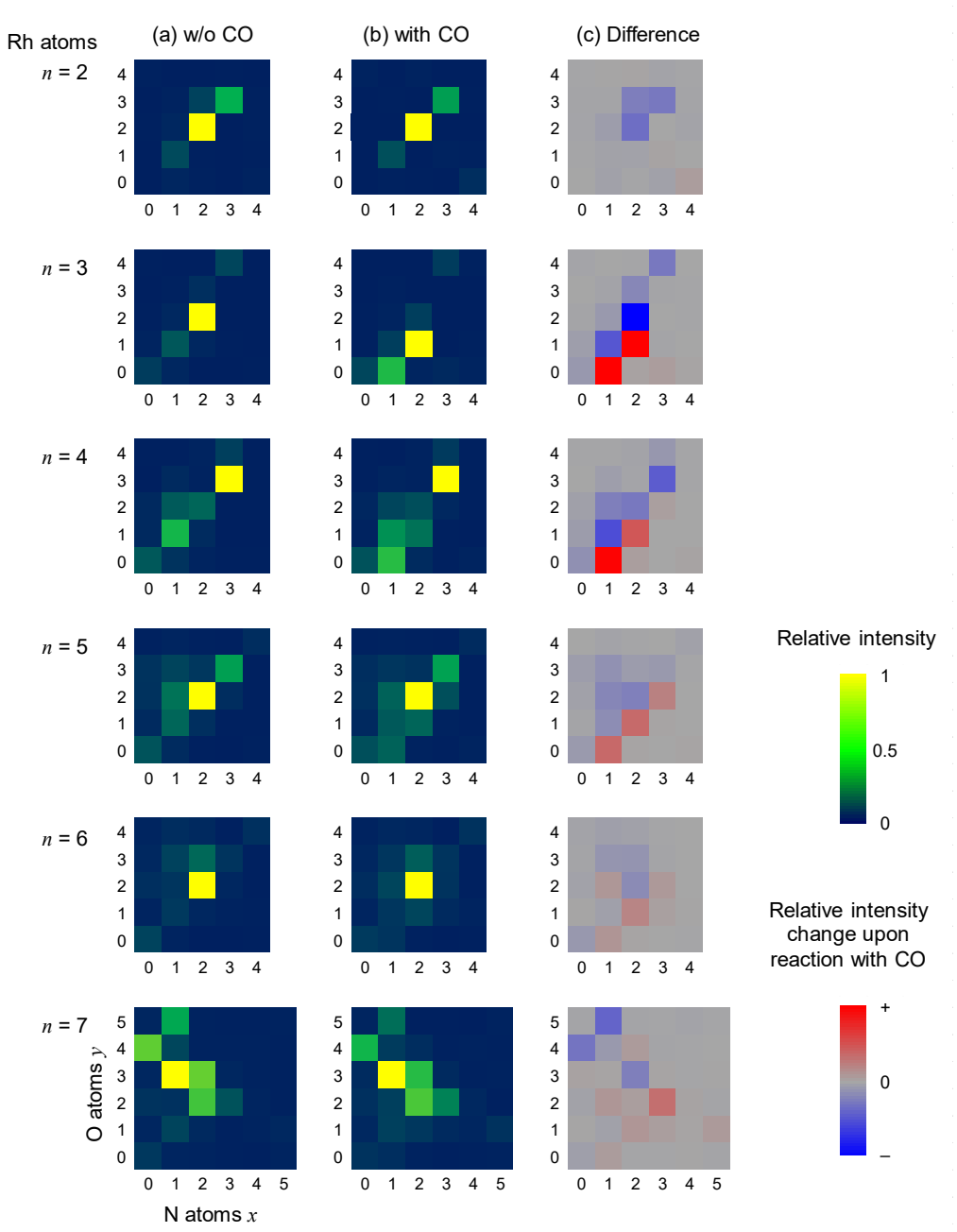


Fig. S4 Signal intensity of $Rh_{2-7}N_xO_y^+$ cluster ions after heating in an extension tube at 903 K. (a) without CO gas reactant, (b) with CO gas reactant, and (c) the difference between them. To minimize the fluctuation, the average value of four measurements was used. Blue and red colors indicate a decrease and increase in response to CO gas injection, respectively, and gray indicates no changes.

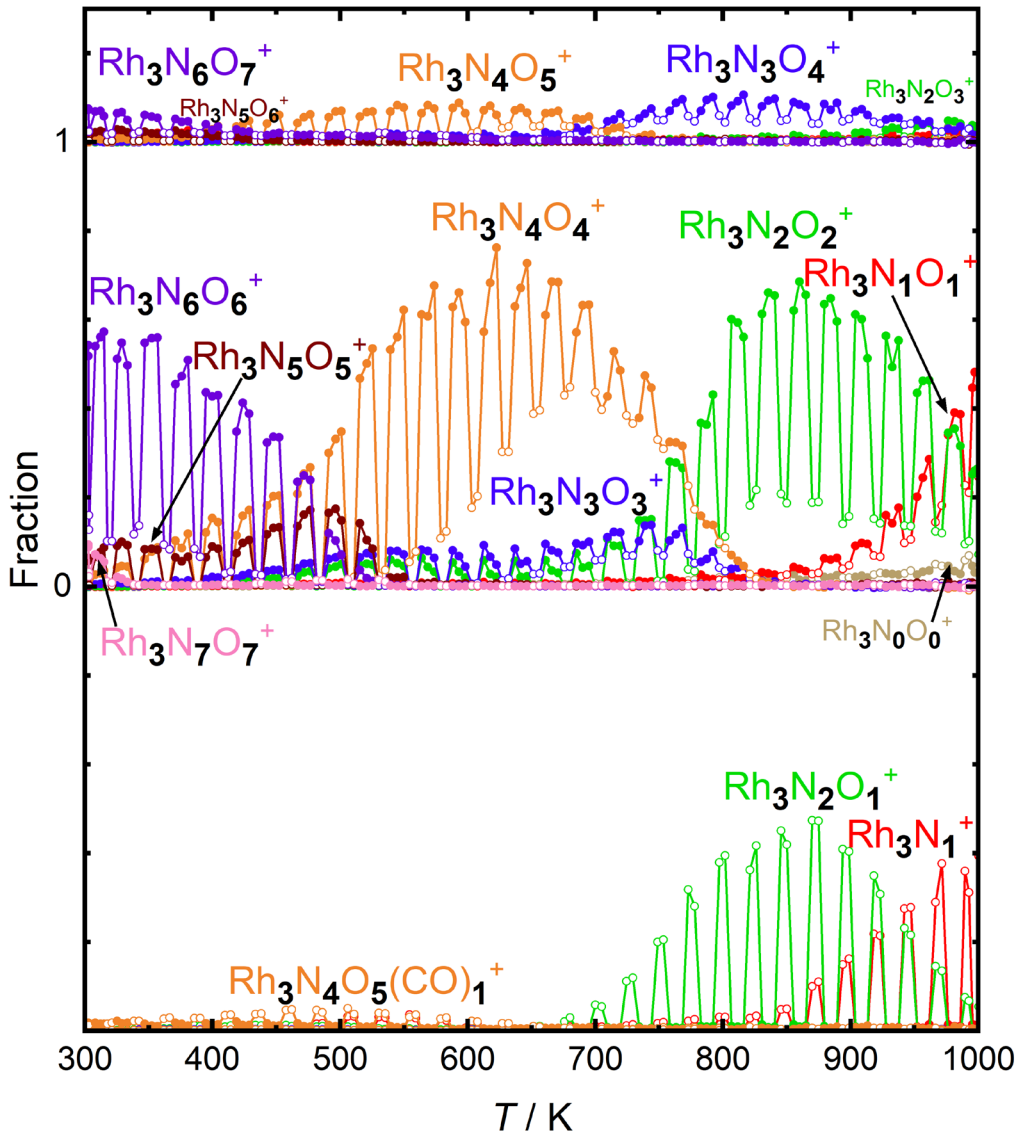


Fig. S5 TDS plots for $n = 3$ with alternate on–off gas injection of CO. The cluster ions, $Rh_3N_xO_y^+$, grouped with the same y-x value (y-x = +1 – -1) are shown from top to bottom. Even when a CO molecule is presumed to be originally attached, our mass resolution cannot distinguish it from two N atoms attached. Here, for the purpose of plotting in one figure, a cluster with k CO molecules attached is categorized as if the cluster had $2k$ N atoms instead of the k CO molecules. The number of nitrogen atoms in the cluster is color-coded as red, green, blue, orange, brown, purple, and pink.

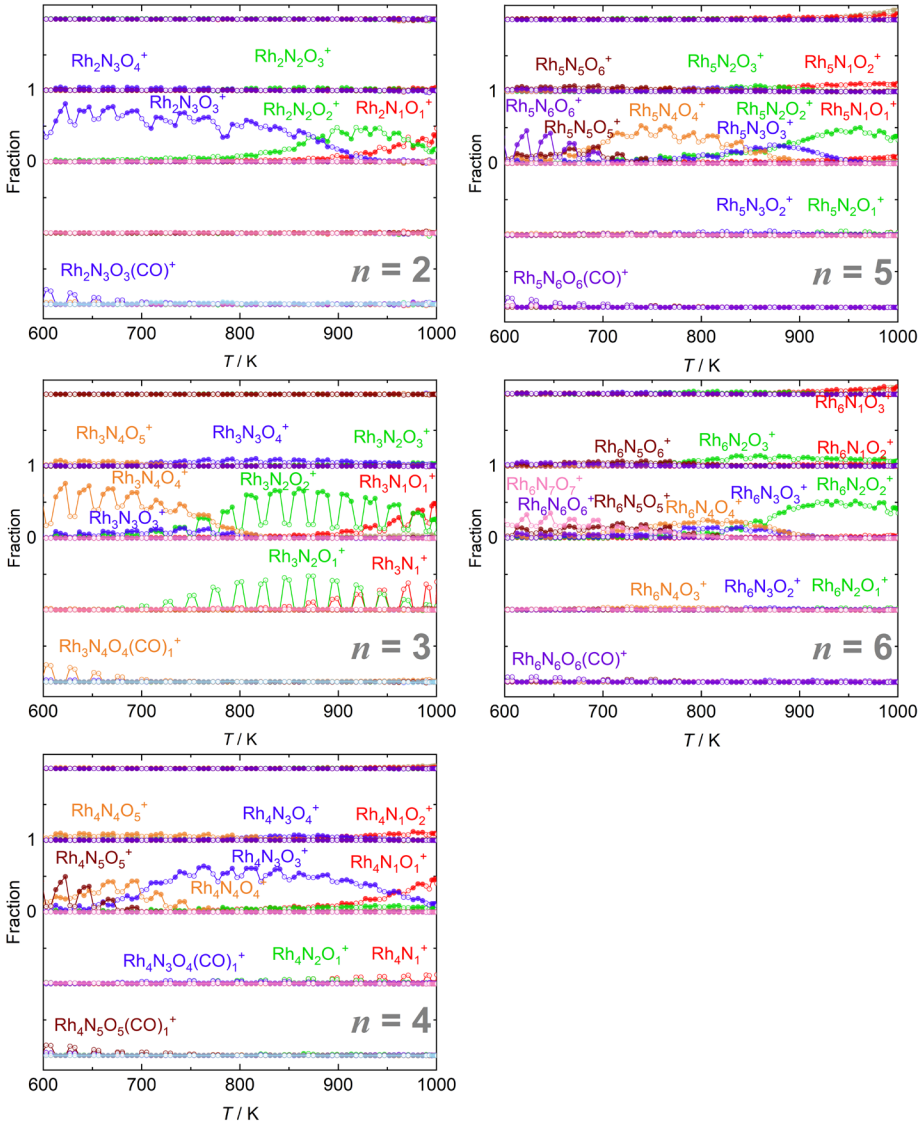


Fig. S6 TDS plots for n = 2–5 with alternate on–off gas injection of CO. The cluster ions, $Rh_nN_xO_y^+$, grouped with the same y-x value (y-x = +2 – -2) are shown from top to bottom. Even when a CO molecule is presumed to be originally attached, our mass resolution cannot distinguish it from two N atoms attached. Here, for the purpose of plotting in one figure, a cluster with k CO molecules attached is categorized as if the cluster had 2k N atoms instead of the k CO molecules. In the alternate on–off gas injection of CO, the intensities of the clusters produced in the presence and absence of CO are depicted by open and filled circles, respectively. The number of nitrogen atoms in the cluster is color-coded as red, green, blue, orange, brown, purple, and pink.

For $n = 4$, the thermal desorption of NO occurred as follows:

$Rh_4N_xO_x^+ \rightarrow Rh_4N_{x-1}O_{x-1}^+ + NO$ ($x = 2–5$),

$Rh_4N_xO_{x+1}^+ \rightarrow Rh_4N_{x-1}O_x^+ + NO$ ($x = 2–4$).

The reduction by CO proceeds as follows:

$Rh_4N_xO_{x+1}^+ + CO \rightarrow Rh_4N_xO_x^+ + CO_2$ ($x = 1–4$),

$Rh_4N_xO_x^+ + CO \rightarrow Rh_4N_xO_{x-1}^+ + CO_2$ ($x = 1–5$).

For $n = 5$, the thermal desorption of NO occurred as follows:

$Rh_5N_xO_x^+ \rightarrow Rh_5N_{x-1}O_{x-1}^+ + NO$ ($x = 2–6$),

$Rh_5N_xO_{x+1}^+ \rightarrow Rh_5N_{x-1}O_x^+ + NO$ ($x = 2–5$).

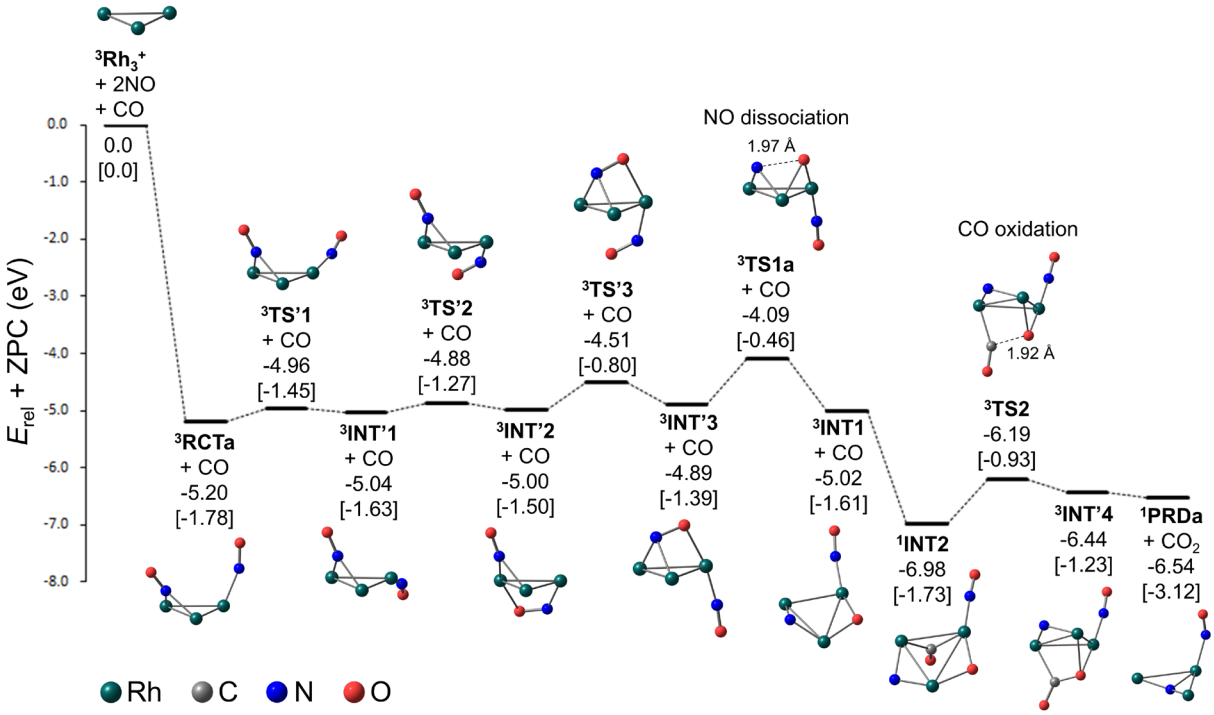
The reduction by CO proceeds as follows:

$Rh_5N_xO_{x+1}^+ + CO \rightarrow Rh_5N_xO_x^+ + CO_2$ ($x = 1–5$),

$Rh_5N_xO_x^+ + CO \rightarrow Rh_5N_xO_{x-1}^+ + CO_2$ ($x = 1–4$).

For $n = 2$, $Rh_2N_xO_x^+$ adsorbed a CO molecule on $Rh_2N_3O_3^+$ below 700 K and sequentially desorbed NO molecules above 700 K. In addition, the intensities of $Rh_2N_3O_4^+$ and $Rh_2N_2O_3^+$ decreased when the CO gas was on, although the changes were not as prominent.

(A) Reaction route via **^{3}TS1a** of NO dissociation



(B) Reaction route via **^{3}TS1b** of NO dissociation

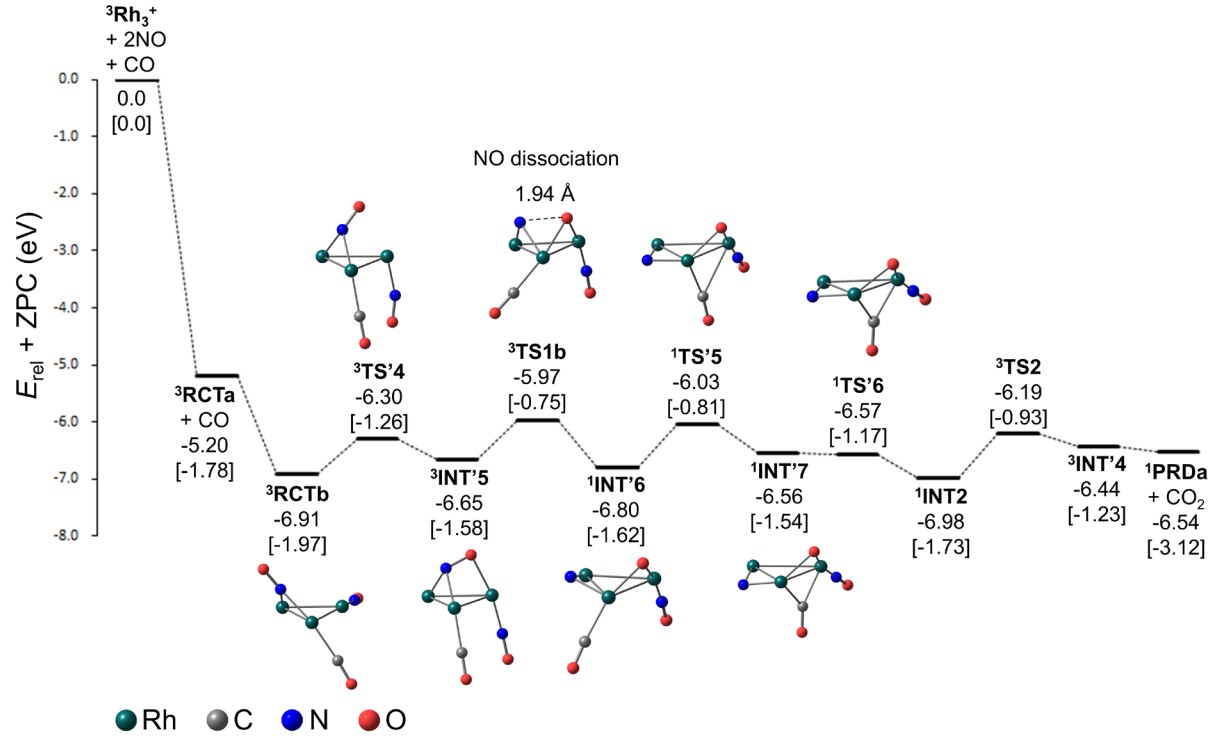
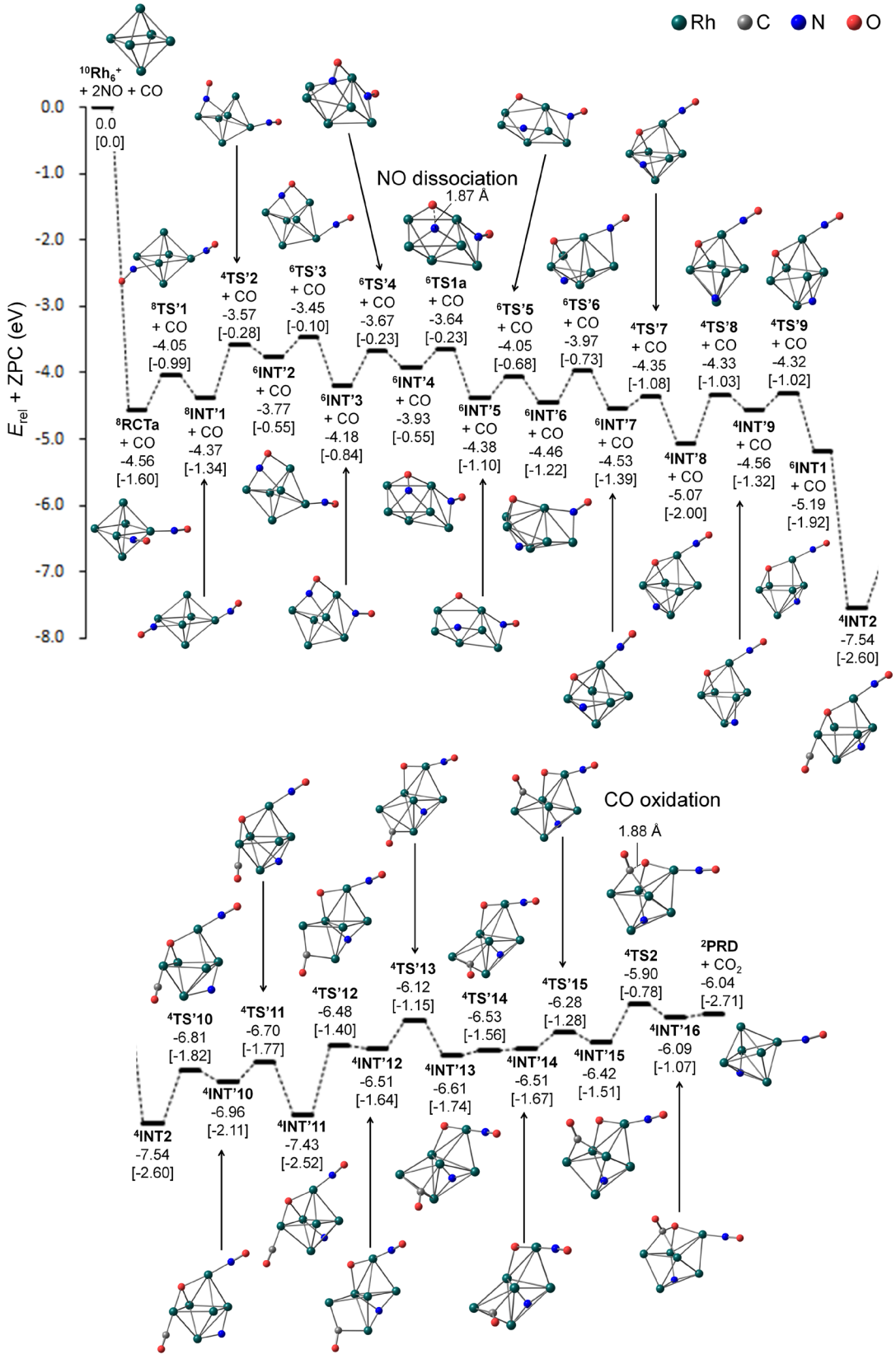


Fig. S7 Overall zero-point corrected energy profiles for the reduction of $Rh_3N_2O_2^+$ by CO calculated at the TPSSh-D3/def2-TZVP//def2-SV(P) level using the RI technique. **RCT**, **INT**, **PRD**, and **TS** represent the reactant, intermediate, product, and transition state, respectively. Superscripts on the labels indicate the values of spin multiplicity. Energy levels are given relative to the sum of energies of the bare Rh cluster, 2NO, and CO. Relative Gibbs free energy (T = 903 K, P = 0.04 atm) is also shown in square brackets.

(A) Reaction route via **^{6}TS1a** of NO dissociation



(B) Reaction route via **^{6}TS1b** of NO dissociation

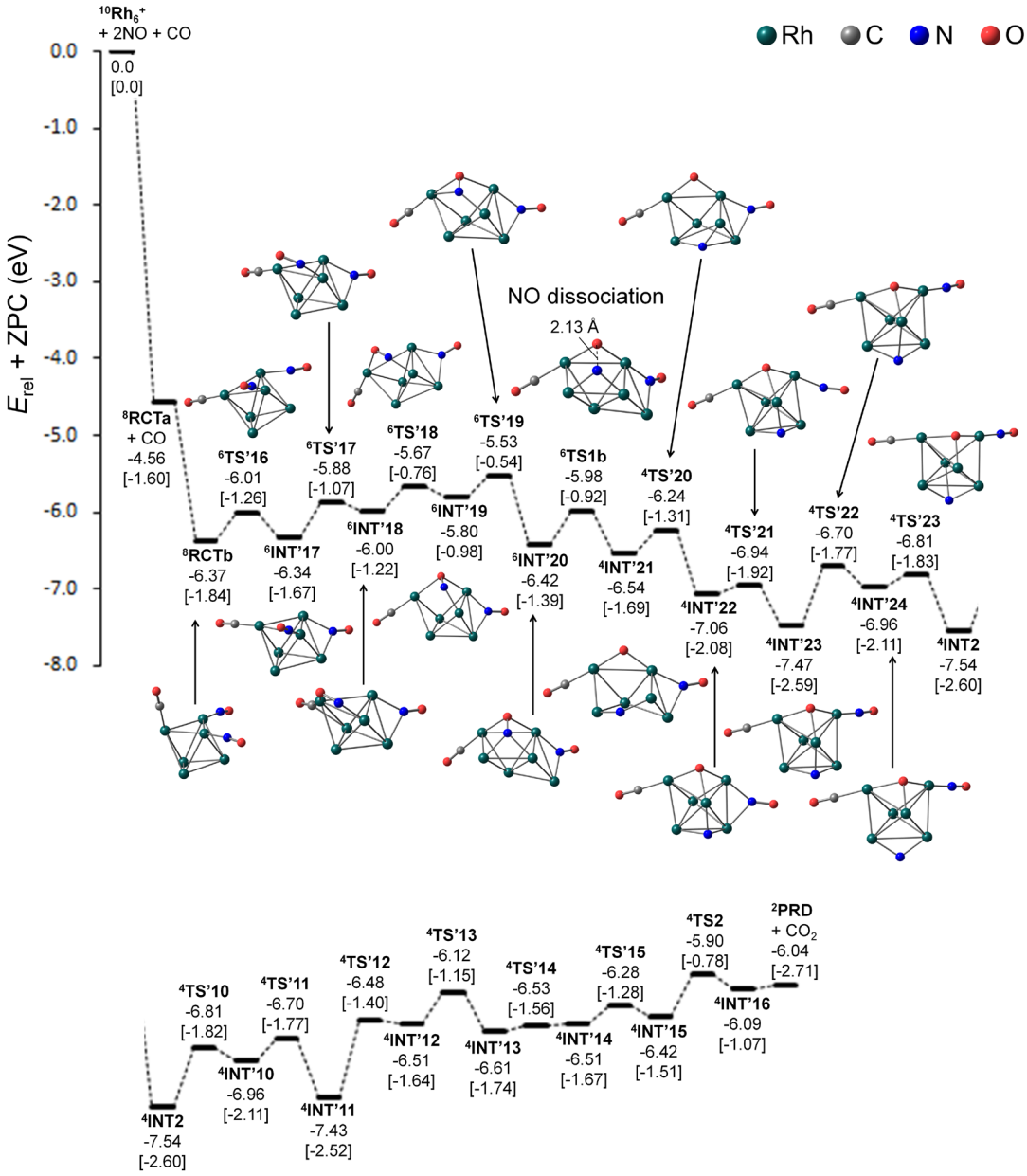


Fig. S8 Overall zero-point corrected energy profiles for the reduction of $Rh_6N_2O_2^+$ by CO were calculated at the TPSSh-D3/def2-TZVP//def2-SV(P) level using the RI technique. **RCT**, **INT**, **PRD**, and **TS** represent the reactant, intermediate, product, and transition state, respectively. Superscripts on the labels indicate the values of spin multiplicity. Energy levels are given relative to the sum of energies of the bare Rh cluster, 2NO, and CO. Relative Gibbs free energy (T = 903 K, P = 0.04 atm) is also shown in square brackets.

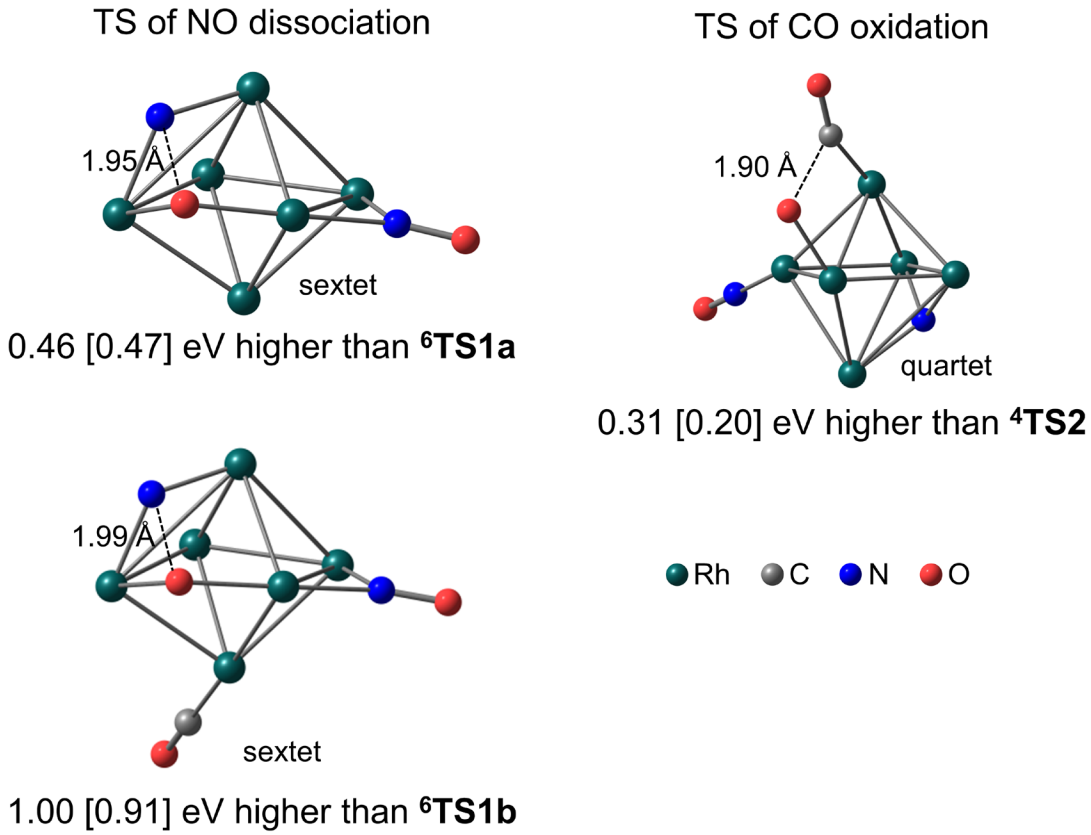


Fig. S9 Octahedral Rh_6 structures at transition states for NO dissociation and CO oxidation and relative stability with zero-point corrected energy. Relative Gibbs free energy (T = 903 K, P = 0.04 atm) is also shown in square brackets.

Optimized structures and energies determined at the RI-TPSSh-D3/def2-SV(P) level

The reduction of $Rh_3N_2O_2^+$ by CO (Fig. S7)

・**$^3Rh_3^+$**

2S + 1 = 3

Rh	1.125341041456	0.828515004958	0.077952224569
Rh	0.171163440151	-1.362149545773	-0.569001835643
Rh	-1.296504481607	0.533634540813	0.491049611077

ENERGY = -331.185472660160 hartree

(A) Reaction route via **^{3}TS1a** of NO dissociation

・**^{3}RCTa**

2S + 1 = 3

Rh	-1.610282247498	0.335251797184	-0.629829456542
Rh	-0.318441625204	-0.995956682929	1.295841804758
Rh	0.249189447406	1.402249369867	0.712592965365
O	2.560124095779	1.228160558207	-0.953891907410
N	1.769905806605	1.550060268752	-0.191397978515
O	-0.465537337750	-2.157910681635	-1.265269889183
N	-0.670638686392	-1.275261849496	-0.515564346243

ENERGY = -590.965087078240 hartree

・**^{3}TS'1**

2S + 1 = 3

Rh	1.423599299598	-1.480811819985	-0.197679153640
Rh	0.780422397128	1.019109219334	0.359644560838
Rh	-0.221218131310	-0.947390006272	1.626005211763
O	0.130176428851	0.038566489751	-2.206247517657
N	0.551944252955	-0.111825400966	-1.120935954725
O	-2.785398276091	-0.257439975631	2.826771590081
N	-1.720963107298	-0.530806611003	2.523803900085

ENERGY = -590.955698394720 hartree

・**^{3}INT'1**

2S + 1 = 3

Rh	1.586615507212	-1.408544157192	-0.065543097308
Rh	0.580916948354	0.978642060626	0.381219821065

Rh	-0.535133207550	-1.043554180003	1.333941924798
O	0.500527607991	-0.024594927153	-2.283213446400
N	0.753963915806	-0.173135451086	-1.147540240130
O	-1.787737159398	0.170648143904	3.640229658247
N	-1.509973304808	-0.389816160905	2.685153529452

ENERGY = -590.959818801550 hartree

・**^{3}TS'2**

2S + 1 = 3

Rh	1.613407020412	-0.878801382110	0.149336650101
Rh	-0.467127221243	0.709774399868	0.316067473953
Rh	-0.613086186608	-1.565246839533	1.335788249335
O	0.378867466602	-0.162093994745	-2.280449673397
N	0.466015200720	-0.176841920684	-1.110829736682
O	-1.670029971876	0.470414889842	2.813794427071
N	-1.549483444175	-0.667803257411	2.587655246354

ENERGY = -590.954931440470 hartree

・**^{3}INT'2**

2S + 1 = 3

Rh	1.579480121007	-0.481615636463	0.250539679010
Rh	-0.526202896597	0.862040100430	0.292725168775
Rh	-0.806037591490	-1.572750795278	1.028507104905
O	0.758318901401	0.406467650925	-2.320318000491
N	0.601736370895	0.383763597102	-1.163625033643
O	-1.530008177666	0.651825465017	2.195830496419
N	-1.470217465881	-0.542146207690	2.355297090722

ENERGY = -590.958058169380 hartree

・**^{3}TS'3**

2S + 1 = 3

Rh	1.641706441754	-0.391016398619	0.401710829593
Rh	-0.504679309123	1.046937061922	0.279372841569
Rh	-0.808360645113	-1.491538709787	0.672318080909
O	-0.086915726900	-0.984347701099	-1.355191316367
N	0.439026167009	0.108928797412	-1.071020818677
O	-1.260695962548	0.277863332050	2.619097052705
N	-1.262366334174	-0.838116136007	2.266885349625

ENERGY = -590.939279267710 hartree

・**^{3}INT'3**

2S + 1 = 3

Rh	1.627549472084	-0.360776705759	0.433283558764
Rh	-0.407119091254	1.138556723314	-0.002570679666
Rh	-0.866632485833	-1.339985890831	0.745882940858
O	-0.147753357574	-1.177227707670	-1.182385736187
N	0.488249666910	-0.067293397845	-1.153050714819
O	-1.473201891482	-0.944598936613	3.537087814711
N	-1.294449367094	-1.180588639655	2.438235297541

ENERGY = -590.950102885160 hartree

・**^{3}TS1a of NO dissociation step**

2S + 1 = 3

Rh	1.708640672150	-0.325440617473	0.207707874327
Rh	-0.356689252472	1.333594296028	-0.244960326629
Rh	-0.838494098253	-1.021035229447	0.663067024440
O	0.263499408343	-1.435267976475	-0.814256920089
N	0.774132098965	0.418134941279	-1.229024964944
O	-1.868172940482	-0.169506033278	3.248553815580
N	-1.570512994248	-0.533843043632	2.212169502319

ENERGY = -590.909440503660 hartree

・**^{3}INT1**

2S + 1 = 3

Rh	1.488534966377	0.324717082776	0.105878723218
Rh	-0.096655684949	-1.551799531845	-1.147001285499
Rh	-0.997255292317	0.731475639578	0.768461998789
O	-1.589430809176	-0.579783197411	-0.431594493200
N	1.312762848346	-0.539834746461	-1.389649909904
O	-0.812004106673	3.553599282310	1.407540308381
N	-0.793820150608	2.419452091053	1.296417840217

ENERGY = -590.943416492590 hartree

・**^{3}INT2**

2S + 1 = 1

Rh	1.289249248256	-0.150355884742	1.239921144446
Rh	1.160159253892	2.219093955208	0.150848327220

Rh	-1.097581658525	0.213301306559	-0.069433553210
O	-0.579727218112	1.940017631694	-0.607576059265
N	2.376498412414	1.264678082680	0.867558666765
O	-2.691427082991	-2.221507906900	0.213251393116
N	-2.062462516566	-1.275317870696	0.161246440374
O	1.077428703641	-1.272723783532	-1.469427236486
C	0.648345735993	-0.717185530271	-0.544351154959

ENERGY = -704.241261679980 hartree

・^{3}TS2 of CO oxidation step

2S + 1 = 3

Rh	0.756264415058	-1.399115417389	0.247663993609
Rh	0.075217653933	1.519008427737	-0.300428345132
Rh	-1.383672933596	-0.500305020570	-1.121976941240
O	0.144428799301	0.411319879196	-1.941124068236
N	0.819266175446	0.331468911336	0.764096262380
O	-3.623229798059	-1.207432825753	0.580446021569
N	-2.768512176330	-0.999708566017	-0.141770461455
O	1.929705145146	-1.365704920686	-2.532543897532
C	1.301448581104	-1.088442889859	-1.610144168955

ENERGY = -704.221247242400 hartree

・^{3}INT'4

2S + 1 = 3

Rh	0.789722986870	-1.399306335144	0.202327217377
Rh	0.027733799757	1.492022803833	-0.285612202783
Rh	-1.377775673360	-0.522099054172	-1.114875302432
O	0.354420938445	0.224899894681	-2.032412621148
N	0.692137147427	0.263511640795	0.817231599688
O	-3.606106591623	-1.024151146017	0.655860047155
N	-2.796944485111	-0.821945819477	-0.118554476185
O	1.985841268874	-1.355963360764	-2.368777887289
C	1.175129585839	-0.805433804867	-1.695537616565

ENERGY = -704.237092808460 hartree

・^{1}PRD1

2S + 1 = 1

Rh	1.042562532898	-0.032340282990	0.081292216992

Rh	0.944995594080	2.091183925900	2.532111055505
Rh	-0.772448098939	2.217269069161	0.197083313527
N	0.821701414123	1.477425682133	0.911972130781
O	-3.095890380049	0.963754146328	1.187594676448
N	-2.452316182111	1.691894806466	0.577640265746

ENERGY = -515.795229429760 hartree

(B) Reaction route via **^{3}TS1b** of NO dissociation

・**^{3}RCTb**

2S + 1 = 3

Rh	1.368857811164	-1.105148041110	0.291850742096
Rh	-0.112873104238	-0.023966553768	-1.590850110067
Rh	-0.976454071732	-0.340173067073	0.767760123805
O	2.564689105766	1.135605110336	-0.828209714161
N	1.618706420588	0.448401709885	-0.778162716308
O	-1.343501628325	-1.491952031374	3.419866477061
N	-1.295508178307	-0.954102172454	2.416879988206
O	-2.555780466600	-1.693533942421	-2.411748158444
C	-1.679546964070	-1.034452451292	-2.096213595346

ENERGY = -704.256258579230 hartree

・**^{3}TS'4**

2S + 1 = 3

Rh	1.544115408304	-1.519803193607	0.023088335989
Rh	-0.258676908772	-0.356092140361	-1.421947084366
Rh	-0.111708161657	0.195769223921	1.257708545493
O	1.825692662420	1.203536885234	-0.057987809044
N	1.484187631632	0.202991245090	-0.646596211483
O	-2.008345844959	-1.817326761882	1.993143245407
N	-1.341115701957	-0.899928616794	1.865187298016
O	-2.870601690317	-1.959030299979	-1.478726390979
C	-1.910676475985	-1.342878491913	-1.524576677727

ENERGY = -704.232817776890 hartree

・**^{1}INT'5**

2S + 1 = 3

Rh	1.578771822636	-1.528543736324	-0.019269556400

Rh	-0.265442645734	-0.356525337151	-1.425816628794
Rh	-0.070727570588	0.185920486962	1.251905450600
O	1.421989495650	1.103310121214	0.217472648584
N	1.517790627405	0.215057066878	-0.688936803046
O	-2.128176130917	-1.591879691706	2.224668533233
N	-1.313794708696	-0.874338540290	1.888196748935
O	-2.853020797726	-1.989157897298	-1.602889644353
C	-1.909350643032	-1.346531021285	-1.601630272758

ENERGY = -704.243230963500

・**^{3}TS1b**

2S + 1 = 3

Rh	0.878504833538	-1.919926679189	0.051749258071
Rh	-0.817029627395	-0.043491740262	-1.015534492590
Rh	0.138994897657	-0.019893108444	1.594342228130
O	0.601862638459	0.976153111459	0.061482167785
N	0.994324759031	-0.593965708432	-1.102322001331
O	-1.267191273201	-1.675744990588	3.532285287440
N	-0.628971905913	-1.017711281874	2.857914953370
O	-2.530310146017	-2.092594687278	-2.533656727899
C	-1.918326917154	-1.308163828392	-1.979032783976

ENERGY = -704.207072257880 hartree

・**^{1}INT'6**

2S + 1 = 1

Rh	1.023346245559	-1.886973373918	-0.241857727622
Rh	-0.545208989451	-0.047076637621	-1.317598628215
Rh	-0.048441640189	-0.030070443686	1.419604935003
O	0.303704055257	1.082367548747	-0.019584108440
N	0.834559253340	-1.188000069314	-1.778487371652
O	-1.229734556419	-1.964165460162	3.251217411106
N	-0.685788558611	-1.207003779516	2.590153679361
O	-2.709194704441	-1.756457081360	-2.770862816572
C	-1.888242106490	-1.143013945652	-2.282577472754

ENERGY = -704.234924065090 hartree

・**^{1}TS'5**

2S + 1 = 1

Rh	1.196443143270	-1.966770163360	-0.425681586533
Rh	-0.184054541648	0.031268762513	-1.369885328817
Rh	-0.465750294378	-0.048851251108	1.249291098057
O	0.160461430804	1.285536648301	0.148422911150
N	0.815495644249	-1.370315543463	-1.987560859418
O	-1.526798986729	-2.067954051501	3.087027967410
N	-1.098572873633	-1.289747644227	2.369782926102
O	-2.701282479228	-1.576060788008	-0.806876207748
C	-1.755547356637	-0.941805203192	-0.890545641451

ENERGY = -704.205763471610 hartree

・**^{1}INT'7**

2S + 1 = 1

Rh	1.050255196050	-1.983006882593	-0.517579496736
Rh	-0.144545759187	0.139252061341	-1.460894485948
Rh	-0.500118731768	-0.216184847877	1.258684910274
O	0.214859043594	1.156826300875	0.183376400723
N	0.593081800048	-1.388235213892	-2.060762155990
O	-1.838101306352	-1.764705699111	3.352380870295
N	-1.268499201512	-1.204583606716	2.541823112436
O	-2.507914867069	-1.436771404857	-0.586525164882
C	-1.558124875551	-0.837320928469	-0.295347804245

ENERGY = -704.226720588340 hartree

・**^{1}TS'6**

2S + 1 = 1

Rh	0.965775992707	-1.997770301900	-0.511576296729
Rh	-0.102163563231	0.169913915592	-1.473671542469
Rh	-0.505076797715	-0.200007885001	1.264915930281
O	0.088449075485	1.214030891741	0.180203529755
N	0.708293570497	-1.308704468929	-2.071770276015
O	-1.746673018433	-1.770188716816	3.401993087291
N	-1.215039796249	-1.211273422573	2.565632649408
O	-2.341227447469	-1.625351278466	-0.621667018443
C	-1.417556497546	-0.991277692113	-0.312357010229

ENERGY = -704.226462316210 hartree

The reduction of $Rh_6N_2O_2^+$ by CO (Fig. S8)

・**$^{10}Rh_6^+$**

2S + 1 = 10

Rh	-1.120815059854	1.129585470686	0.872602282306
Rh	-0.704281439759	-1.403909755394	0.911836627429
Rh	1.121978655783	-1.130372451882	-0.874032940789
Rh	-1.241296056260	-0.224276143089	-1.302640116730
Rh	0.701620296871	1.402453884167	-0.911897290320
Rh	1.242793603218	0.226518996512	1.304131437102

ENERGY = -662.847356943540 hartree

(A) Reaction route via **^{6}TS1a** of NO dissociation

・**^{8}RCTa**

2S + 1 = 8

Rh	-1.326060208705	0.462002009217	-0.748182096430
Rh	-1.263616205710	-0.410608688709	1.664172363482
Rh	-0.804518013096	-2.072827737410	-0.150795392996
Rh	1.176161074705	-1.083968659924	1.314225988225
Rh	1.058614089639	-0.367091292904	-1.141435808718
Rh	0.484869961809	1.330243351049	0.837090709187
O	0.088834280776	-3.868777515709	-2.275291858934
N	-0.362509140479	-3.230037015663	-1.435976809811
O	2.969659521778	1.428425448582	-2.387465822088
N	2.237498914290	0.618325426479	-2.023547105912

ENERGY = -922.595595959430 hartree

・**^{8}TS'1**

2S + 1 = 8

Rh	-1.605538801870	0.893003621325	-0.920996442645
Rh	-1.057357098911	-1.549573667235	-0.050284130797
Rh	-0.346604119737	-0.764106663497	-2.446306489705
Rh	1.450760765379	-1.017966491758	-0.563466580354
Rh	0.870545281316	1.367533974637	-1.594009473887
Rh	0.109420679382	0.724171336173	0.835139112586
O	-0.900063162612	-4.450450868616	-0.308160644913
N	-1.017963335997	-3.319568357309	-0.140567908964

O	3.698711242157	0.758557498737	-0.356311892138
N	2.868548704914	0.097700214903	-0.831542366588

ENERGY = -922.577012397540 hartree

· ^{8}INT'1

2S + 1 = 8

Rh	-1.669395922866	0.863325915294	-0.914914399809
Rh	-1.132658159219	-1.601739789754	-0.036461521360
Rh	-0.318203129029	-0.739851434697	-2.350825102285
Rh	1.437160616775	-0.966552609515	-0.496261951594
Rh	1.045731553170	1.318376612485	-1.542723983971
Rh	0.022352691004	0.753291801091	0.793141360636
O	-0.829056266340	-4.454052368761	-0.490616529862
N	-1.002702811173	-3.355733010638	-0.199745662305
O	3.819997932286	0.757697667340	-0.828724405660
N	2.714062911165	0.432629186088	-1.053929988893

ENERGY = -922.589598165960 hartree

· ^{4}TS'2

2S + 1 = 4

Rh	-1.375037010466	1.024090191593	-0.603732489585
Rh	-1.069904055683	-1.098198327043	0.863415313318
Rh	0.449489103295	-0.587810743432	-1.133175989651
Rh	1.681390264858	0.252609889981	0.885820430453
Rh	0.696883200848	2.394864281709	-0.088753706886
Rh	-0.529068374312	1.140347106698	1.846408162597
O	-2.921904804514	-3.163711307965	0.029205542203
N	-2.043587032507	-2.494138491499	0.344712234201
O	2.586086745020	1.033532481335	-1.574555539334
N	2.377113789850	1.498033131888	-0.481893260873

ENERGY = -922.561052609470 hartree

· ^{6}INT'2

2S + 1 = 6

Rh	-0.973230234137	0.329144036540	-1.173193746767
Rh	-0.694754947692	-1.835165011216	0.233117943341
Rh	0.917710822329	-1.202914187184	-1.650127040458
Rh	1.977625566842	-0.357531414183	0.494387565437

Rh	1.025094791372	1.825543016919	-0.521345475867
Rh	-0.293209196144	0.476415143880	1.276569935273
O	-2.662441372078	-3.790857511807	-0.563399401103
N	-1.763353810969	-3.132181943648	-0.285186207432
O	2.403801616805	0.100352517488	-2.151990704929
N	2.536654686852	0.772519042936	-1.092106932205

ENERGY = -922.567550622510 hartree

・**^{6}TS'3**

2S + 1 = 6

Rh	-1.031777300965	0.473799727280	-1.092330288459
Rh	-0.947765939918	-1.656486877210	0.429842950946
Rh	0.675345746558	-1.278732646609	-1.579376890691
Rh	1.885827135399	-0.481614409075	0.449468114968
Rh	1.137617057516	1.771806691616	-0.579605257427
Rh	-0.223511615152	0.641484688257	1.334823827789
O	-1.074316376934	-4.035237726453	-1.271498680243
N	-0.976333086378	-3.042498867124	-0.690589278990
O	2.295429616932	-0.128457087663	-2.186839535155
N	2.524867473579	0.542559175442	-1.146518855434

ENERGY = -922.555807462400 hartree

・**^{6}INT'3**

2S + 1 = 6

Rh	-1.055163544530	0.399647694810	-1.056700167194
Rh	-0.813725588715	-1.633324056658	0.623565830962
Rh	0.729346004530	-1.309809126440	-1.831006857410
Rh	1.709785388417	-0.613423542436	0.476971658645
Rh	1.119575914756	1.684646925164	-0.607403633441
Rh	-0.283969061874	0.794730098819	1.373639627744
O	-1.042982547937	-3.510781466166	-1.267445362231
N	-0.522862880067	-2.464759756644	-1.046899890020
O	2.452438374488	-0.099535374066	-2.126138278426
N	2.516816433090	0.418798006510	-0.983547301551

ENERGY = -922.585304441100 hartree

・**^{6}TS'4**

2S + 1 = 6

Rh	-0.845348868738	0.809671262383	-1.693963109813
Rh	-0.129471397064	-2.328618853677	1.075793094410
Rh	0.545288198659	-1.400778620170	-1.578109903443
Rh	1.821861326459	-0.578672601582	0.540697144001
Rh	1.142647829496	1.792089294136	-0.475839724648
Rh	-0.708514804402	0.147945865987	0.700749982149
O	-1.464776195648	-3.353215967782	-1.042095181253
N	-0.632088421359	-2.574549542381	-0.702268617214
O	2.205912764372	-0.132904847906	-2.144302230863
N	2.324747267442	0.423382374245	-1.029759851900

ENERGY = -922.568534322470 hartree

・**^{6}INT'4**

2S + 1 = 6

Rh	-0.206827572208	1.138456692054	-2.120962080153
Rh	-0.275329256354	-2.214192188378	1.209208732837
Rh	0.388034567630	-1.518546699620	-1.510916429986
Rh	1.829363401440	-0.729450118393	0.462688564370
Rh	1.274162810998	1.814948952227	-0.106975966611
Rh	-0.667942444348	0.127072450555	0.245498063136
O	-1.261073553721	-3.741791575624	-0.823092315097
N	-0.577767735754	-2.812386161146	-0.532694880392
O	1.624700988820	0.134016130901	-2.180250942020
N	2.205551002559	0.444344605347	-1.037338320011

ENERGY = -922.577834609340 hartree

・**^{6}TS1a** of NO dissociation

2S + 1 = 6

Rh	-0.181533728484	1.081852744405	-2.107700446441
Rh	-0.302997004634	-2.238258085873	1.137968449173
Rh	0.405791648949	-1.499907529206	-1.475316761401
Rh	1.896986151911	-0.811670844968	0.469155797704
Rh	1.213490686139	1.923617635800	-0.174304133329
Rh	-0.638181748951	0.172748661813	0.302884515267
O	-1.372489271652	-3.758800192484	-0.841733541087
N	-0.651700888867	-2.856621588249	-0.580447957928
O	1.408174385022	0.028775205756	-2.262174842209

N	2.271243028566	0.554043869004	-0.684724023750

ENERGY = -922.557848488990 hartree

・^{6}INT'5

2S + 1 = 6

Rh	-0.177268142074	1.220741951105	-2.142057330846
Rh	-0.294095691274	-2.232942744112	1.118179267658
Rh	0.327558449001	-1.593080354816	-1.466311635447
Rh	1.890084124206	-0.935823818470	0.493121333596
Rh	1.220696741446	2.060477382699	-0.201919352747
Rh	-0.562701839664	0.195524291102	0.245063102575
O	-1.184967080005	-4.036336488613	-0.718033026621
N	-0.577830712098	-3.036515026382	-0.554754245802
O	1.000410736703	-0.152905174671	-2.512167506463
N	2.280211807048	0.729524899735	0.157964943775

ENERGY = -922.580398461890 hartree

・^{6}TS'5

2S + 1 = 6

Rh	-0.608178591191	1.125435937301	-2.004415626951
Rh	-0.451036283018	-2.247486516740	1.091038989815
Rh	0.331901709215	-1.449248013162	-1.417315775580
Rh	1.835335519129	-1.012663963021	0.689464010977
Rh	1.489638765968	1.830987225610	-0.606246531623
Rh	-0.511806980907	0.253696962368	0.388805582123
O	-1.018269777964	-4.015669792620	-0.909512413861
N	-0.513816530248	-2.981078887960	-0.638893520956
O	0.959031631541	0.117822462409	-2.373453062193
N	2.347703880959	0.580855314480	0.234159951161

ENERGY = -922.568644072740 hartree

・^{6}INT'6

2S + 1 = 6

Rh	-0.890368541740	1.159866975607	-2.032253533511
Rh	-0.600346934626	-1.966036734902	1.120809862485
Rh	0.195652860898	-1.269161059160	-1.347788835682
Rh	1.775871499156	-0.768394050128	0.917395359644
Rh	1.723748077206	1.100592916250	-0.934788439944

Rh	-0.545743271712	0.531204011652	0.398808102872
O	-1.348109793990	-3.695377275927	-0.911686207142
N	-0.765776100141	-2.720654862530	-0.599007712937
O	0.790166339867	0.216160755189	-2.523506243128
N	2.474007305968	0.831347096199	0.632023489086

ENERGY = -922.581565508610 hartree

・^{6}TS'6

2S + 1 = 6

Rh	-1.145387014235	0.916350312687	-1.811369259516
Rh	-0.840892967391	-1.567581236825	0.887053497503
Rh	0.302015547533	-1.363859069828	-1.485799822549
Rh	1.681881603973	-0.886709945041	0.960731810852
Rh	1.800817703480	1.016930918778	-0.925674485529
Rh	-0.382243712423	0.829493505222	0.558899542312
O	-0.390704036876	-4.147199360492	-0.953912653885
N	-0.161847759497	-3.015412216422	-1.005689131992
O	0.634293793702	0.303665998986	-2.436651355578
N	2.632849589899	0.539954569394	0.542865593138

ENERGY = -922.562760929690 hartree

・^{6}INT'7

2S + 1 = 6

Rh	-1.350179242776	0.549168870832	-1.370845771883
Rh	-1.123238415299	-1.173974233370	0.548454406148
Rh	0.471611664019	-1.548001770923	-1.555904452402
Rh	1.444725970519	-0.913867455606	0.950087697542
Rh	1.848230946799	0.946200805229	-0.990065770548
Rh	-0.070517670252	1.204944556131	0.754930269667
O	0.628324539925	-4.442395146079	-1.506983258688
N	0.554324076507	-3.298501899816	-1.473462032527
O	0.365620357603	0.312324250164	-2.236347354501
N	2.684870277254	0.226965523331	0.368616140445

ENERGY = -922.585562347330 hartree

・^{4}TS'7

2S + 1 = 4

Rh	-1.175748877513	1.166900667988	-1.248623668831

Rh	-1.255615217026	-0.749632047016	0.459364387508
Rh	0.319991384368	-1.610685853546	-1.464794482621
Rh	1.330540674697	-1.025388362163	0.965491060494
Rh	1.682323440135	0.992602791054	-1.071312794543
Rh	0.155550680348	1.328722436115	0.978057435258
O	0.189740122191	-4.471779966928	-1.041058387708
N	0.272042930853	-3.340204721448	-1.204124336586
O	0.168359067064	0.226655567268	-2.223217001174
N	2.400860956896	0.288673306549	0.386360014525

ENERGY = -922.579832752910 hartree

・**^{4}INT'8**

2S + 1 = 4

Rh	-1.074877280434	1.154643189358	-1.249490908395
Rh	-1.240784565425	-0.767935158212	0.437380318886
Rh	0.273441935148	-1.674778608742	-1.507891360531
Rh	1.367172672533	-0.961669045536	0.864037236177
Rh	1.681689873899	0.936089169495	-1.109892692128
Rh	0.138360310164	1.372173536089	1.141323408688
O	0.122030238292	-4.528168571222	-1.021413869798
N	0.201785306825	-3.395594150582	-1.187352359830
O	0.189393316263	0.129783648057	-2.266622542898
N	1.883075782239	0.831694138250	0.705164195639

ENERGY = -922.606872310030 hartree

・**^{4}TS'8**

2S + 1 = 4

Rh	1.308681865667	0.785098596040	-0.688523547360
Rh	-0.010280393599	-1.278615127092	-0.110788857997
Rh	-0.810435486771	0.563943580127	1.594515803029
Rh	-2.446525172159	-0.464053116468	-0.306602646866
Rh	-1.196241597743	1.754725421885	-0.994301726453
Rh	-0.435699374647	-0.284558376893	-2.523878912301
O	-1.541238194221	-1.196183078344	3.781971735997
N	-1.296241332650	-0.492837363959	2.907916417774
O	0.195965890515	1.834518553142	0.461369770551
N	-2.144509205390	-0.273303077438	-2.041775918383

ENERGY = -922.578662926070 hartree

・^{4}INT'9

2S + 1 = 4

Rh	1.338238657414	0.777544905873	-0.773551145459
Rh	0.049723447423	-1.245260721667	-0.072654055980
Rh	-0.817488095635	0.535416568111	1.622157498315
Rh	-2.421043421674	-0.416174362772	-0.361108560013
Rh	-1.201619608327	1.811730836695	-0.957262416694
Rh	-0.498499992008	-0.286706118047	-2.470308168053
O	-1.729315809156	-1.231193438546	3.732181021713
N	-1.420886909399	-0.519888695210	2.886495984416
O	0.229719630210	1.719023480172	0.463874972773
N	-2.127956521147	-0.799473220616	-2.055055000607

ENERGY = -922.587162059530 hartree

・^{4}TS'9

2S + 1 = 4

Rh	1.477830090644	0.673754786646	-0.679109311820
Rh	-0.150925537646	-1.330270450318	-0.200451537612
Rh	-0.297916945093	0.433262567879	1.752782142585
Rh	-2.321008595067	0.145304979111	-0.028691080911
Rh	-0.987044490515	2.070480056446	-0.944895823018
Rh	-0.452548185684	0.009164912195	-2.449748993150
O	-1.288232474133	-1.380583566312	3.781517335223
N	-0.878776801549	-0.655013604543	2.994459767645
O	0.301225906179	1.790897365987	0.468368476957
N	-1.936330701136	-0.548930389089	-1.641357147900

ENERGY = -922.579805893010 hartree

・^{6}INT1

2S + 1 = 6

Rh	1.445083074928	0.934979686998	-1.977064964808
Rh	-0.446016029391	-0.601955581034	1.009601384398
Rh	-0.294846239037	-1.799837930245	-1.319081838559
Rh	2.128480565300	-1.127113789934	-0.573044385508
Rh	1.540563022669	1.630949650118	0.523304583729
Rh	-0.787920063864	1.391859709372	-0.602382558072

O	-0.391285572956	-4.587637335813	-0.551717898652
N	-0.362047061779	-3.486825178611	-0.869642700629
O	-0.320866141163	0.051224444653	-1.975488178963
N	1.326551958290	-0.176353103504	0.779626045061

ENERGY = -922.617522729550 hartree

・**^{4}INT2**

2S + 1 = 4

Rh	-0.996102928039	0.232433641151	1.538895806013
Rh	0.967460372581	-0.396112204756	-1.963495936712
Rh	2.006320587565	0.383767542061	0.319569328972
Rh	0.471923969806	-1.730390933856	0.723517582656
Rh	-1.857969350657	-0.331460499546	-0.741354366664
Rh	-0.432329905510	1.634633480139	-1.284648789263
O	4.581352297830	-0.934859167240	0.372338870712
N	3.577548829270	-0.382030874334	0.343788709964
O	0.312711514831	1.376126570733	0.483510283983
N	-0.257356747082	-1.272733826595	-0.905380094145
O	-2.971329673730	-1.520589354502	2.980901603513
C	-2.223239518656	-0.838801960612	2.437202522131

ENERGY = -1035.934702255830 hartree

・**^{4}TS'10**

2S + 1 = 4

Rh	0.091248051075	-0.766716156222	1.074847867508
Rh	-0.322132163315	0.034495968152	-2.415108962048
Rh	1.738092354990	0.841022214923	-0.222438447968
Rh	1.150205299497	-1.622622352589	-1.200088024549
Rh	-1.852348579178	-1.160777711935	-0.703293278824
Rh	-1.379068304139	1.202922281046	0.233640027693
O	4.152963543198	0.143302553615	1.217574251141
N	3.214161340388	0.424502049553	0.624357523409
O	0.124365280083	1.422843945468	-1.144392370152
N	-0.462532913272	-2.268012488304	-0.799698030886
O	-3.537778741996	0.791520481802	2.292204239641
C	-2.728318305617	0.947090682573	1.491261617806

ENERGY = -1035.900016811760 hartree

・**^{4}INT'10**

2S + 1 = 4

Rh	0.119689027014	-0.671921198732	1.100803669473
Rh	-0.332198162478	0.179122833124	-2.290446372730
Rh	1.819784169937	0.803712869126	-0.256260507236
Rh	1.054179369352	-1.646197236151	-1.169711650057
Rh	-1.781511462427	-1.263136803722	-0.605130021338
Rh	-1.433673810318	1.192193440250	0.168221348824
O	4.297579864288	-0.033242607373	0.984746452873
N	3.330388918006	0.279963548277	0.455926835827
O	0.187018002628	1.555531377022	-1.015725075719
N	-0.543680805530	-2.400362089075	-1.124411982143
O	-3.866509073446	0.628897585852	1.859270070191
C	-2.950575497818	0.831285604556	1.195822845832

ENERGY = -1035.904362700520 hartree

・**^{4}TS'11**

2S + 1 = 4

Rh	0.112001615380	-0.570594144458	1.155001510863
Rh	-0.225723625218	-0.032054129165	-2.327420210018
Rh	1.753858275556	0.779997697120	-0.328767164324
Rh	1.125726356815	-1.812454757541	-0.926085143091
Rh	-1.824866349624	-1.217240825319	-0.566251086633
Rh	-1.410469090157	1.203453320328	0.209421038676
O	4.147206190816	0.213096572618	1.214555936856
N	3.232138514786	0.398239264640	0.545732742921
O	0.136396665958	1.539894381913	-1.017631786435
N	-0.552484902205	-2.199149377615	-1.298035252471
O	-3.549580108520	0.768501941480	2.294189403600
C	-2.748922617735	0.922784447893	1.483733916859

ENERGY = -1035.894970874530 hartree

・**^{4}INT'11**

2S + 1 = 4

Rh	0.308044257349	-0.858134134963	1.871371683470
Rh	-0.198051408311	-0.018408596355	-1.735624061221
Rh	1.913294012430	0.518943504041	0.303461773168

Rh	1.126996106605	-1.977147061374	-0.382405400857
Rh	-1.472391668782	-1.561179361826	0.030835552061
Rh	-1.173465934098	0.950976922040	0.795318559744
O	4.450264640541	-0.214773846403	1.503372429329
N	3.441223541579	0.032147815561	1.017948410666
O	0.367620263073	1.438962488578	-0.390441108435
N	-0.377981150633	-1.825277967812	-1.488994371427
O	-3.567504956361	0.383485745070	2.544238046449
C	-2.651686601251	0.571890617151	1.874875895234

ENERGY = -1035.925648110000

・**^{4}TS'12**

2S + 1 = 4

Rh	0.243308574729	-0.660347077886	1.425899990993
Rh	-0.348517517668	0.013720584043	-1.053405614369
Rh	2.234353145330	0.471601149493	0.188382002977
Rh	1.336262028503	-2.016403191408	-0.529484779791
Rh	-1.761956474448	-1.778338779115	0.235879491499
Rh	-1.293259218018	1.312678019948	0.865000856508
O	4.453676965958	-0.418933429435	1.838671572872
N	3.582490247384	-0.141284645273	1.148348027835
O	0.913820229193	1.463324260180	-0.740945036350
N	-0.409463740192	-1.880474464492	-1.072919541109
O	-3.621526939900	-0.460761388035	1.431086929240
C	-2.608562362649	-0.014356865980	1.016686887160

ENERGY = -1035.884061727730 hartree

・**^{4}INT'12**

2S + 1 = 4

Rh	0.265048111760	-0.523065401626	1.408055091198
Rh	-0.338571716958	0.067234946512	-1.040087117246
Rh	2.338345826901	0.404717358676	0.145398589571
Rh	1.295007925836	-2.016596497052	-0.553610587385
Rh	-1.718027611838	-1.809907306091	0.247973083813
Rh	-1.444064306390	1.301965401583	0.915894837818
O	4.364035833786	-0.526287652915	2.015367248171
N	3.575053053539	-0.213385879977	1.245873533701

O	1.118848464408	1.307798214954	-0.971200744237
N	-0.430017622016	-1.818503925377	-1.120314423544
O	-3.643734432770	-0.569020212916	1.470134091484
C	-2.633930274517	-0.150010821906	1.011881157692

ENERGY = -1035.885050954910 hartree

・**^{4}TS'13**

2S + 1 = 4

Rh	0.098842122737	-0.232873570485	1.284246442722
Rh	-0.170133550443	0.251914773703	-1.314942956656
Rh	2.338489650251	0.380317951249	0.084396513356
Rh	1.167146189822	-2.004646736321	-0.419531906639
Rh	-1.767996416366	-1.703994084358	0.028793936023
Rh	-1.902282965701	1.142492187530	0.352822232771
O	4.203831451484	-0.568355849892	2.111041153514
N	3.471885733684	-0.269602747675	1.279592116004
O	1.325348592830	1.447411804624	-1.084122053870
N	-0.404880948762	-1.598312848988	-1.282652336920
O	-3.148512558217	-0.576829824595	2.335618583572
C	-2.491112363087	-0.377096882757	1.377939063622

ENERGY = -1035.872976759370 hartree

・**^{4}INT'13**

2S + 1 = 4

Rh	-0.057540658836	-0.077207884970	1.046954806378
Rh	-0.289991553080	0.356308115244	-1.387914820390
Rh	2.398619328324	0.366302523507	0.039191971327
Rh	1.120856632708	-1.966835682376	-0.374439604909
Rh	-1.820587310255	-1.644693803048	-0.416113518044
Rh	-2.371120928647	0.876459749383	0.220367749904
O	3.823084383855	-0.701313648635	2.338483011269
N	3.293196806159	-0.318756952992	1.397088312027
O	1.412802440271	1.211344513830	-1.328224004575
N	-0.272807901437	-1.527015968047	-1.483253243014
O	-2.556567656128	-1.047779578755	2.421950332757
C	-1.969168798793	-0.564722698498	1.512634652128

ENERGY = -1035.889184861820 hartree

・**^{4}TS'14**

2S + 1 = 4

Rh	-0.085938827984	-0.209448500737	1.023636094755
Rh	-0.198226336626	0.205343029477	-1.421008600074
Rh	2.361595656606	0.442243971152	0.140716915376
Rh	1.182099249432	-1.903260526551	-0.556917623345
Rh	-1.889285199523	-1.609070646788	-0.443259421891
Rh	-2.392054318286	0.854412059498	0.242587502206
O	3.855498302461	-0.652107676568	2.384964825778
N	3.275224426583	-0.240747236771	1.487087705062
O	1.386481943790	1.238272147016	-1.266573512285
N	-0.398065420950	-1.678107094267	-1.511069191856
O	-2.413417716331	-0.443824601466	2.853955598277
C	-1.963286820970	-0.113280751960	1.819080495514

ENERGY = -1035.884288457150 hartree

・**^{4}INT'14**

2S + 1 = 4

Rh	-0.089772897311	-0.117159241299	0.947848481190
Rh	-0.140036197305	0.213869741010	-1.515638202413
Rh	2.402151195200	0.406133657711	0.175622399715
Rh	1.165493383494	-1.864840781931	-0.594387720062
Rh	-1.887331517606	-1.603231779617	-0.446164665499
Rh	-2.506885631018	0.756670863713	0.339315353015
O	3.606085637878	-0.672359305385	2.595174508738
N	3.165378426728	-0.244508344118	1.628302511724
O	1.525608468115	1.109277641429	-1.345303543206
N	-0.438355220973	-1.660022321283	-1.537285582686
O	-2.124438162115	-0.291140381823	3.056980748113
C	-1.908310892026	-0.006933246100	1.938395653128

ENERGY = -1035.885005016780 hartree

・**^{4}TS'15**

2S + 1 = 4

Rh	-0.300631439200	-1.258416954265	1.263395492016
Rh	-0.356564351446	0.304364952433	-1.514028495529
Rh	1.691711502843	0.329278905918	0.640566428474

Rh	1.233784459795	-1.721140515454	-0.981636558865
Rh	-1.551490090357	-2.205302919502	-0.887411401472
Rh	-2.337931435785	0.056869880197	0.129477426067
O	3.625948075437	-0.794948056656	2.509069058465
N	2.853763755975	-0.404319293975	1.755243199312
O	0.658698355751	1.503127623997	-0.380957870847
N	-0.275747299227	-1.505566957761	-2.039892167093
O	-1.242386435520	1.183545482219	2.566250172849
C	-1.278530160064	0.402932024878	1.693125504110

ENERGY = -1035.876865350430 hartree

・**^{4}INT'15**

2S + 1 = 4

Rh	-0.278966257213	-1.249559015035	1.311885703663
Rh	-0.301591823654	0.448773120561	-1.539005660776
Rh	1.726923103169	0.304616563931	0.678845222482
Rh	1.092479499552	-1.639386385104	-1.023103194229
Rh	-1.573210858474	-2.340998728835	-0.766318251755
Rh	-2.249699231395	-0.016206604527	-0.012349592551
O	3.677317660739	-0.881247195150	2.485817469231
N	2.895924821632	-0.462698408924	1.756109908449
O	0.713972873392	1.540634050145	-0.306895463908
N	-0.510927245210	-1.389110927368	-1.957738341695
O	-1.381029053653	1.193255351892	2.480383709425
C	-1.319558227402	0.386963811814	1.633140796160

ENERGY = -1035.884504647940 hartree

・**^{4}TS2** of CO oxidation

2S + 1 = 4

Rh	-0.271574292960	-1.274197034249	1.315886925452
Rh	-0.326946427630	0.440838711144	-1.530603374139
Rh	1.720400943997	0.320620744288	0.725663036076
Rh	1.149742353370	-1.650723142792	-0.971880306273
Rh	-1.536276205293	-2.357313892435	-0.773701322429
Rh	-2.257337171627	-0.057311944987	-0.005304423633
O	3.982008422126	-0.803676661713	2.152344901340
N	3.096116415153	-0.384415437352	1.557977009771

O	0.239413485712	1.417784975489	0.137870998355
N	-0.428312144364	-1.400292426875	-1.908178533016
O	-1.204789430258	1.330160505112	2.269339638394
C	-0.983456513222	0.638507995373	1.335430997103

ENERGY = -1035.869687488160 hartree

・**^{4}INT'16**

2S + 1 = 4

Rh	-0.272025625508	-1.269981962475	1.277890063840
Rh	-0.340465388282	0.428189189092	-1.544389333959
Rh	1.744886056574	0.344813791306	0.742830091385
Rh	1.182853905130	-1.646217344946	-0.940205383261
Rh	-1.563923585472	-2.362706742379	-0.785269949604
Rh	-2.259091818548	-0.064851568960	0.023210298631
O	3.966790443896	-0.937409532794	2.061977084318
N	3.101541375691	-0.431615456658	1.509508931727
O	0.090486880100	1.442111920277	0.319465212604
N	-0.406948100351	-1.414785572217	-1.840809240485
O	-1.285900302704	1.314770391188	2.174877422266
C	-0.864243820254	0.843729525658	1.137268730039

ENERGY = -1035.882421847530 hartree

・**^{2}PRD**

2S + 1 = 2

Rh	1.815512956639	-0.324341116969	-0.804594103457
Rh	-1.013174297486	-0.703817520560	-1.611531454471
Rh	-1.579148736844	0.230893277967	0.743802679554
Rh	0.111938228200	-1.665018207934	0.454729563707
Rh	0.903219643440	0.536456307053	1.415713276308
Rh	-0.116476841513	1.985356892951	-0.478223380459
N	0.337789037990	0.541640149526	-1.513685504543
O	-3.796173562842	1.341595754704	2.271130756437
N	-2.874435878575	1.029898592260	1.655443143921

ENERGY = -847.434268952160 hartree

(B) Reaction route via ^{6}**TS1b** of NO dissociation

・**^{8}RCTb**

2S + 1 = 8

Rh	1.107546807897	1.420153585093	-0.381079836876
Rh	-1.059160586295	1.313542050920	1.078064952445
Rh	0.867027272564	-1.429968983919	-0.598458397686
Rh	-1.208933828188	-1.164331833385	0.918285829120
Rh	-1.053417194396	0.247515537802	-1.268355450420
Rh	1.120641690654	-0.162853052148	1.605717346370
O	0.823609762776	4.035470554641	-1.613576356496
N	1.052947737386	2.980571568252	-1.222530346154
O	0.452375058417	-3.423687437050	-2.681573202161
N	0.679255094135	-2.621349593439	-1.895939782165
O	3.671143546228	-1.817614943225	1.532932412331
C	2.708902050786	-1.192486438827	1.553309662840

ENERGY = -1035.890454813480 hartree

・^{6}TS'16

2S + 1 = 6

Rh	-2.094086262171	-0.725258531594	0.762796648721
Rh	-1.058720164904	1.496133877779	0.059187766767
Rh	0.371190878212	-0.286219331414	1.488741759703
Rh	-0.119852692734	-2.056968542613	-0.343779318287
Rh	-1.366414243091	-0.350142003662	-1.756957637658
Rh	1.050319486544	0.275810306904	-0.928048255440
O	-0.793074341785	4.027981012095	-1.345009169226
N	-0.827381890692	3.046301508276	-0.747818480301
O	-1.112633943240	-1.540390276640	3.682860873625
N	-0.685219466744	-0.937201674093	2.794700443144
O	3.157735755025	-1.767652086373	-1.590421174827
C	2.362231065321	-0.971457979412	-1.352314747298

ENERGY = -1035.877197200100 hartree

・^{6}INT'17

2S + 1 = 6

Rh	-2.134802164235	-0.721838539420	0.882023282678
Rh	-1.001877073719	1.469079765469	0.067228514357
Rh	0.323506948420	-0.279791379663	1.509551645656
Rh	-0.065727154682	-2.011706747226	-0.323602675127

Rh	-1.335404299228	-0.392211807384	-1.737630034215
Rh	1.089537282284	0.277872781065	-0.997328446935
O	-0.843038428189	3.960107936370	-1.425379530859
N	-0.910277388520	2.978252998762	-0.833370023661
O	-1.384775855075	-1.598239404992	3.494090303592
N	-1.123624861213	-1.003286208462	2.512690473642
O	3.128323309565	-1.720477587152	-1.939123505958
C	2.363040319338	-0.937070371984	-1.587480786662

ENERGY = -1035.890556396720 hartree

・**^{6}TS'17**

2S + 1 = 6

Rh	-2.106153424243	-1.107249652927	0.886875064636
Rh	-1.595470479951	1.431291831179	0.018645681605
Rh	0.132277821804	0.096745858640	1.462860004308
Rh	0.239254856491	-1.827417287127	-0.220732894996
Rh	-1.345950721968	-0.503460091499	-1.671316199832
Rh	0.905556195058	0.655968943603	-1.023920320343
O	0.096708175341	2.946756904984	-1.465766522466
N	-0.948831526594	2.781153500207	-0.936034651343
O	-1.265116665717	-1.442176081873	3.543725680296
N	-1.101575307255	-0.879074159721	2.522521263591
O	3.081521238774	-1.349541169855	-1.478610225016
C	2.212542784497	-0.611985290922	-1.281511672775

ENERGY = -1035.874044540770 hartree

・**^{6}INT'18**

2S + 1 = 6

Rh	-2.077652090584	-1.153637612525	0.881004458765
Rh	-1.747250721904	1.439856169665	0.020065683058
Rh	0.069645291305	0.193560465329	1.416035456680
Rh	0.294019005679	-1.810803784852	-0.204852165658
Rh	-1.309033167462	-0.438572767860	-1.636605324484
Rh	1.000503996961	0.664825239061	-1.062727314838
O	0.239446027426	2.679270175103	-1.272058019574
N	-0.884102034051	2.749482569277	-0.834921966330
O	-1.067740162412	-1.537133576845	3.498539631986

N	-1.037988299685	-0.904181299885	2.508188169332
O	2.876615383079	-1.636052303689	-1.441548151702
C	1.986462450810	-0.930399213876	-1.173629044151

ENERGY = -1035.879498175190 hartree

・**^{6}TS'18**

2S + 1 = 6

Rh	-2.023778184546	-1.308086279870	0.755665139260
Rh	-2.066434561850	1.213001578019	-0.155644262605
Rh	-0.152397349581	0.575699095317	1.594705776759
Rh	0.509224508546	-1.435302559374	0.121115371432
Rh	-0.978708092903	-0.487380152443	-1.701296051069
Rh	1.226549851743	0.769922713527	-1.121944485864
O	0.306779422874	2.498245182363	-0.251965440392
N	-0.914375986829	2.548081427360	-0.350868734127
O	-1.552643121069	-0.984735814695	3.499267561805
N	-1.343261700411	-0.618576541096	2.394688647986
O	2.715616271129	-1.458539191717	-2.446803605561
C	2.114235775423	-0.633463259967	-1.911766318574

ENERGY = -1035.870266537920 hartree

・**^{6}INT'19**

2S + 1 = 6

Rh	-1.998525166773	-1.270826285739	0.817740156019
Rh	-2.044028062813	1.194323646832	-0.402814087983
Rh	-0.380817937431	0.756049684046	1.620437667852
Rh	0.600577040464	-1.328035616632	0.382478582518
Rh	-0.866722308958	-0.695359940529	-1.604531584177
Rh	1.263190854910	0.706567952937	-1.075968177956
O	0.351082592955	2.220663043974	0.175984404980
N	-0.721216083516	2.397823575423	-0.487181371579
O	-1.681353654973	-0.964331238376	3.554611931223
N	-1.406535245361	-0.563043032281	2.478822871445
O	2.634014608156	-1.266343595083	-2.853890140411
C	2.091140195857	-0.508621997136	-2.180536652895

ENERGY = -1035.874149094430 hartree

・**^{6}TS'19**

2S + 1 = 6

Rh	-2.007645769837	-1.321145075643	0.963329832698
Rh	-2.211425035661	1.112424457896	-0.224889777431
Rh	-0.426506105283	0.777498156753	1.584981671018
Rh	0.488100595035	-1.272392839571	0.260598245826
Rh	-0.814583677560	-0.494205598777	-1.717137808913
Rh	1.481908113522	0.647420056757	-1.114743219468
O	0.268765906746	2.061854234465	-0.032335729610
N	-0.754648886399	2.020982270660	-0.799171376003
O	-1.701811788757	-0.800174714532	3.669827032276
N	-1.446342146000	-0.494513404182	2.557867771138
O	2.965599900852	-1.409621573003	-2.697329215075
C	2.389469520022	-0.621363238597	-2.090246101709

ENERGY = -1035.865347000060 hartree

・**^{6}INT'20**

2S + 1 = 6

Rh	-2.140140758086	-1.539990135926	1.148458052204
Rh	-2.206370285772	0.592868657899	-0.455156023252
Rh	-0.382392171766	0.733457900198	1.347974762313
Rh	-0.213126040469	-1.172557918986	-0.493192350384
Rh	-0.395435903030	0.563812458466	-2.414815681693
Rh	1.596076255183	0.691342445508	-0.821694949522
O	0.132195583385	2.110453036839	-0.247575841408
N	-0.858261454296	1.841117527709	-1.079866516507
O	-1.033064690368	-0.934807360341	3.567251122338
N	-1.128688856816	-0.617850297122	2.426578529936
O	3.348151013216	-1.508061361962	-1.890617603067
C	2.693246993569	-0.660593107520	-1.476819407925

ENERGY = -1035.898176773460 hartree

・**^{6}TS1b** of NO dissociation

2S + 1 = 6

Rh	-2.094531446156	-1.463342912941	1.284352621590
Rh	-2.198808303613	0.610053197827	-0.580531798162
Rh	-0.486569484051	0.698992539960	1.319888497007
Rh	-0.279298572072	-1.217888942204	-0.501063930093

Rh	-0.303142184837	0.617311700779	-2.460342476360
Rh	1.541660651213	0.648172408078	-0.752272413809
O	0.358907642957	1.936369489481	0.135393681206
N	-1.119186628779	1.822467577181	-1.396077783576
O	-0.764994918032	-1.082293219117	3.661587121320
N	-1.006069775196	-0.653709574416	2.590668346406
O	3.410396121230	-1.329967759590	-2.124735325380
C	2.703578111347	-0.586164500056	-1.613112209132

ENERGY = -1035.868268797140 hartree

・^{4}INT'21

2S + 1 = 4

Rh	-2.269124341219	-0.975108090909	0.781318278459
Rh	-2.334144414435	1.291240124423	-0.448463634187
Rh	-0.476046046190	0.806210082647	1.293571985769
Rh	0.239754215525	-1.262932378327	0.052741795152
Rh	-0.141425092833	-0.120688546522	-2.245835572329
Rh	1.769765232568	0.643223311071	-0.751342428627
O	0.876732002042	1.797409954695	0.546186632532
N	-1.603125467668	0.758380863177	-1.948868173428
O	-1.992358699963	-0.445963641007	3.543343900665
N	-1.671195507586	-0.199573946383	2.440883320445
O	3.466789858416	-1.193892860202	-2.468312423635
C	2.793389548908	-0.503724061804	-1.843133375741

ENERGY = -1035.888050837270 hartree

・^{4}TS'20

2S + 1 = 4

Rh	-2.246568233180	-0.955125006373	0.574377562903
Rh	-2.219750918623	1.465608555637	-0.477441975952
Rh	-0.458230819731	0.769849043976	1.315178711967
Rh	0.378856256622	-1.313420629205	0.169154902085
Rh	-0.251800970389	-0.255858340950	-2.120362826573
Rh	1.690881926821	0.700101414820	-0.755173977733
O	1.002120905646	1.740653233849	0.744579250408
N	-1.863341734862	0.128077290805	-1.581618987612
O	-2.213418777655	-0.436827826827	3.389717532044

N	-1.784694238657	-0.218461656283	2.319245835786
O	3.302861223783	-0.934914106360	-2.736535826391
C	2.638919290971	-0.325087280660	-2.022285718246

ENERGY = -1035.877225523870 hartree

・**^{4}INT'23**

2S + 1 = 4

Rh	-2.080962621049	-1.058144322358	0.401405396592
Rh	-1.404857172748	1.618066796714	-0.676077409659
Rh	-0.527232110675	0.654703313598	1.630079936593
Rh	0.495615736449	-1.195184089748	0.259472826846
Rh	-0.669599821461	-0.480416144269	-2.009553127290
Rh	1.361824969804	0.862408969830	-0.880716259476
O	0.337954130761	1.967791581647	0.406931966322
N	-2.235358116626	0.061654401791	-1.184454467154
O	-2.756173272890	-0.549356384735	3.144539682626
N	-1.921625450249	-0.470476822331	2.318511262632
O	3.139394670561	-0.754438926998	-2.730325543085
C	2.441392654160	-0.158502302328	-2.039226217283

ENERGY = -1035.911691756780 hartree

・**^{4}TS'21**

2S + 1 = 4

Rh	-2.164274636905	-1.012529338707	0.233012438425
Rh	-1.477381730588	1.586487934289	-0.705333773342
Rh	-0.577225520415	0.656796866320	1.641282120747
Rh	0.429876296550	-1.206989504713	0.227088519469
Rh	-0.608920628672	-0.435632137812	-2.098337795416
Rh	1.353243115254	0.839798804900	-0.871981892507
O	0.333721170325	1.888017252324	0.469500489336
N	-2.227606268358	0.026570076180	-1.335681965653
O	-2.675938847432	-0.600969433309	3.264613128728
N	-1.822262371499	-0.332935553130	2.526018794225
O	3.167490430812	-0.754043861675	-2.698810837847
C	2.452309615459	-0.160854699605	-2.022146140774

ENERGY = -1035.905377792080 hartree

・**^{4}INT'23**

2S + 1 = 4

Rh	-2.424697127236	-0.501768649741	-0.366014184256
Rh	-1.351146905069	1.828929768542	-1.006080819722
Rh	-0.786046634860	0.533039641599	1.572012209630
Rh	0.081983447839	-1.295798767691	-0.000244679456
Rh	-0.459915092795	-0.220911580366	-2.390092456325
Rh	1.387091454033	0.691350407985	-0.769670267877
O	0.156363928672	1.745615835575	0.418999801608
N	-2.143177096629	0.446382746458	-1.925598175803
O	-1.704450125130	-1.170859825531	3.738418019109
N	-1.370859623305	-0.507264274427	2.865169945353
O	3.326270516082	-0.960604014257	-2.393998094714
C	2.571644485073	-0.338719361949	-1.791079840678

ENERGY = -1035.923580929800 hartree

・**^{4}TS'22**

2S + 1 = 4

Rh	-2.478141367373	-0.487251919012	-0.299280784633
Rh	-1.402429668981	1.824707893631	-0.974716526140
Rh	-0.788315578012	0.559873010868	1.576479407951
Rh	0.002922952924	-1.293374728517	-0.064043336063
Rh	-0.368112834643	-0.125958795839	-2.438299199913
Rh	1.429961384955	0.669362801477	-0.774624874136
O	0.167475775518	1.710235076974	0.376827607489
N	-2.075750912931	-0.262719955787	-2.001009140597
O	-1.546516373659	-1.171706261400	3.780770265655
N	-1.317616378849	-0.474431111103	2.897798698722
O	3.416161734310	-1.049199697099	-2.262794786011
C	2.648766008529	-0.388308727524	-1.719331105977

ENERGY = -1035.894957210200 hartree

・**^{4}INT'24**

2S + 1 = 4

Rh	-2.336085511398	0.001297457670	-0.127780691473
Rh	-0.458057733726	0.002717212078	-2.356998245537
Rh	-0.450102692986	0.469284665859	1.781422885754
Rh	-0.043849875412	-1.303915668723	-0.118601483269

Rh	-0.942027949852	2.047971105391	-0.748519699872
Rh	1.558882136751	0.612828354969	-0.840486914564
O	0.469435304490	1.657203667252	0.530531601921
N	-2.120554609797	-0.283347511708	-1.859795186443
O	-1.567127269223	-1.270193197237	3.805024509315
N	-1.166948621008	-0.553588579674	3.006398014680
O	3.139365624760	-0.871390201129	-2.938114028431
C	2.523859026647	-0.299356726403	-2.154091074986

ENERGY = -1035.904362007630 hartree

・**^{4}TS'23**

2S + 1 = 4

Rh	-2.384016180683	0.035151093527	-0.040916585185
Rh	-0.399161857108	0.143521596312	-2.396426684457
Rh	-0.376848539447	0.467569042178	1.731367919758
Rh	-0.111256101750	-1.325821844010	-0.192855231423
Rh	-1.108518430333	2.072718581474	-0.821781030661
Rh	1.578230759916	0.556393629752	-0.782884554905
O	0.344266534736	1.690097819970	0.400747541499
N	-1.894123860376	-0.493838163955	-1.672596173315
O	-1.251687452190	-1.336959630183	3.822501403231
N	-0.930612607605	-0.600765467157	3.005717222966
O	3.318853482648	-1.165807700124	-2.535160648292
C	2.652827227252	-0.499805447561	-1.876990192789

ENERGY = -1035.900051176540 hartree