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Supporting Information for

Catalytic Reduction Mechanism of NO by CO on Rh_4^+ Cluster: A Density Functional Theory Study

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Table S1: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^4Rh_4^+$ + 2NO for all the species in the reaction of Rh_4^+ + 2NO → $O_bRh_4^+$ + N_2O at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
NO	-0.01553	-129.94980	
$^2Rh_4^+$	-0.03392	-442.03091	31.1
$^4Rh_4^+$	-0.03524	-442.04276	
$^4Rh_4^+$ + 2NO	-0.06630	-701.94236	0.0
$^6Rh_4^+$	-0.03569	-442.04175	
$^6Rh_4^+$ + 2NO	-0.06675	-701.94135	2.7
$^3Rh_4^+$NO	-0.03063	-572.03114	
$^3Rh_4^+$NO	-0.03185	-572.03861	
$^3Rh_4^+$NO + NO	-0.04739	-702.22804	-120.9
$^5Rh_4^+$NO	-0.03207	-572.03834	
$^5Rh_4^+$NO + NO	-0.04760	-701.98814	-120.2
^{3}b-Rh_4^+NO	-0.02561	-572.04835	
^{3}b-Rh_4^+NO	-0.02809	-572.04910	
^{3}b-Rh_4^+NO + NO	-0.04362	-701.99890	-148.4
^{5}b-Rh_4^+NO	-0.02900	-572.05799	
^{5}b-Rh_4^+NO + NO	-0.04453	-702.00779	-171.8
^{3}bb-Rh_4^+NO	-0.02943	-572.02544	
^{3}bb-Rh_4^+NO + NO	-0.04497	-701.97524	-86.3
^{5}bb-Rh_4^+NO	-0.03041	-572.02764	
^{5}bb-Rh_4^+NO + NO	-0.04594	-701.97744	-92.1
^{3}TS1-1	-0.03301	-571.94000	
^{3}TS1-1 + NO	-0.04854	-701.88980	138.0
^{5}TS1-1	-0.03269	-571.94734	
^{5}TS1-1 + NO	-0.04822	-701.89714	118.7
$^3NRh_4^+O$	-0.03270	-571.94531	
$^3NRh_4^+O$ + NO	-0.04823	-701.89511	124.1
$^5NRh_4^+O$	-0.03455	-571.95907	

$^{5}NRh_4^+O$ + NO	-0.05008	-701.90887	87.9
$^{7}NRh_4^+O$	-0.03507	-571.95044	
$^{2}NRh_4^+O(NO)$	-0.02815	-701.96487	-59.1
$^{4}NRh_4^+O(NO)$	-0.02870	-701.96732	-65.5
$^{6}NRh_4^+O(NO)$	-0.03107	-701.95197	
$^{2}ONRh_4^+NO$	-0.02868	-702.03483	-242.8
$^{4}ONRh_4^+NO$	-0.02843	-702.04077	-258.4
$^{2}(NO)_bRh_4^+(NO)_b$	-0.02162	-702.06876	-331.9
$^{4}(NO)_bRh_4^+(NO)_b$	-0.02733	-702.06137	-312.5
$^{2}ONRh_4^+(NO)_b$	-0.02433	-702.05220	-288.4
$^{4}ONRh_4^+(NO)_b$	-0.02592	-702.05994	-308.7
$^{6}ONRh_4^+(NO)_b$	-0.02837	-702.04228	
^{2}TS1-2	-0.02840	-701.95246	-26.5
^{4}TS1-2	-0.02776	-701.94966	-19.2
$^{2}NRh_4^+O(NO)_b$	-0.02777	-701.96322	-54.8
$^{4}NRh_4^+O(NO)_b$	-0.02856	-701.96631	-62.9
^{2}TS1-3	-0.02770	-701.95300	-27.9
^{4}TS1-3	-0.02829	-701.96400	-56.8
^{6}TS1-3	-0.03010	-701.95231	
$^{2}NRh_4^+O_b(NO)$	-0.02593	-701.99903	-148.8
$^{4}NRh_4^+O_b(NO)$	-0.02960	-701.98552	-113.3
^{2}TS1-4	-0.02704	-701.99044	-126.2
^{4}TS1-4	-0.02724	-701.98582	-114.1
$^{2}N_bRh_4^+O_b(NO)$	-0.02702	-702.02276	-211.1
$^{4}N_bRh_4^+O_b(NO)$	-0.02807	-702.02179	-208.5
^{2}TS1-5	-0.02634	-701.96161	-50.5
^{4}TS1-5	-0.02869	-701.95912	-44.0
$^{2}ON_2Rh_4^+O_b$	-0.02148	-702.00543	-163.2
$^{4}ON_2Rh_4^+O_b$	-0.02300	-702.00291	-159.0
N_2O	-0.01024	-184.73455	
$^{4}O_bRh_4^+$	-0.03180	-571.27881	

$^4O_bRh_4^+ + N_2O$	-0.04204	-702.01335	-186.4
$^6O_bRh_4^+$	-0.03373	-571.28939	
$^6O_bRh_4^+ + N_2O$	-0.04398	-702.02393	-214.2
$^8O_bRh_4^+$	-0.03467	-517.27713	
^{2}TS1-6	-0.02826	-701.91190	80.0
^{4}TS1-6	-0.02934	-701.91484	72.3
$^2(N)_2Rh_4^+(O)_2$	-0.02764	-701.93501	19.3
$^4(N)_2Rh_4^+(O)_2$	-0.02814	-701.93521	18.8

Table S2: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^4Rh_4^+ + N_2O$ for all the species in the reaction of $Rh_4^+ + N_2O \rightarrow O_bRh_4^+ + N_2$ at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
N_2O	-0.01024	-184.73455	
$^4Rh_4^+$	-0.03524	-442.04276	
$^4Rh_4^+ + N_2O$	-0.04548	-626.77731	0.0
$^6Rh_4^+$	-0.03569	-442.04175	
$^6Rh_4^+ + N_2O$	-0.04593	-626.77629	2.7
$^4Rh_4^+ON_2$	-0.02711	-626.75486	58.9
$^6Rh_4^+ON_2$	-0.02793	-626.76136	41.9
$^4Rh_4^+N_2O$	-0.02744	-626.74895	74.5
$^6Rh_4^+N_2O$	-0.02732	-626.76221	39.7
^{4}TS2-1	-0.02982	-626.75360	62.2
^{6}TS2-1	-0.02940	-626.75506	58.4
^{8}TS2-1	-0.03053	-626.75582	
$^4ORh_4^+N_2$	-0.03205	-626.82264	-119.0
$^6ORh_4^+N_2$	-0.03222	-626.82912	-136.0
$^8ORh_4^+N_2$	-0.03322	-626.83767	
$^2ORh_4^+$	-0.03416	-517.23893	
$^4ORh_4^+$	-0.03537	-517.25755	
$^4ORh_4^+ + N_2$	-0.04825	-626.83391	-148.6
$^6ORh_4^+$	-0.03494	-517.24794	
$^6ORh_4^+ + N_2$	-0.04782	-626.82430	-123.4
^{2}TS2-2	-0.03396	-517.23916	
^{4}TS2-2	-0.03470	-517.25632	
^{4}TS2-2 + N_2	-0.04758	-626.83268	-145.4
^{6}TS2-2	-0.03548	-517.24747	
^{6}TS2-2 + N_2	-0.04835	-626.82383	-122.1
$^4O_bRh_4^+$	-0.03180	-517.27881	

$^4O_bRh_4^+ + N_2$	-0.04468	-626.85517	-204.4
$^6O_bRh_4^+$	-0.03373	-517.28939	
$^6O_bRh_4^+ + N_2$	-0.04661	-626.86575	-232.2

Table S3: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^6O_bRh_4^+$ + CO for all the species in the reaction of $O_bRh_4^+$ + CO → Rh_4^+ + CO_2 at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
CO	-0.01408	-113.36610	
$^6O_bRh_4^+$	-0.03373	-517.28939	
$^6O_bRh_4^+$ + CO	-0.04782	-630.65548	0.0
$^4O_bRh_4^+$	-0.03180	-517.27881	
$^4O_bRh_4^+$ + CO	-0.04588	-630.64490	27.8
$^2O_bRh_4^+$CO	-0.02681	-630.68275	
$^4O_bRh_4^+$CO	-0.02737	-630.68681	-82.2
$^6O_bRh_4^+$CO	-0.02962	-630.67079	-40.2
^{2}TS3-1	-0.02534	-630.64162	
^{4}TS3-1	-0.02788	-630.64827	18.9
^{6}TS3-1	-0.02787	-630.64029	39.9
$^4Rh_4^+CO_2$	-0.02865	-630.68023	-65.0
$^6Rh_4^+CO_2$	-0.02836	-630.68395	-74.8
CO_2	-0.00969	-188.66033	
$^4Rh_4^+$	-0.03524	-442.04276	
$^4Rh_4^+$ + CO_2	-0.04493	-630.70309	-125.0
$^6Rh_4^+$	-0.03569	-442.04175	
$^6Rh_4^+$ + CO_2	-0.04538	-630.70208	-122.3

Table S4: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^4Rh_4^+$ + NO + CO for all the species in the reaction of $^4Rh_4^+$ + NO + CO → $N_bRh_4^+$ + CO_2 at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
NO	-0.01553	-129.94980	
CO	-0.01408	-113.36610	
$^4Rh_4^+$	-0.03524	-442.04276	
$^4Rh_4^+$ + NO + CO	-0.06485	-685.35866	0.0
$^6Rh_4^+$	-0.03569	-442.04175	
$^6Rh_4^+$ + NO + CO	-0.06530	-685.35764	2.7
$^3(ON)_bRh_4^+CO$	-0.02374	-685.45677	-257.6
$^5(ON)_bRh_4^+CO$	-0.02660	-685.45061	-241.4
$^3ONRh_4^+CO$	-0.02811	-685.43961	-212.5
$^5ONRh_4^+CO$	-0.02702	-685.44565	-228.4
$^7ONRh_4^+CO$	-0.02962	-685.44613	
^{3}TS4-1	-0.02458	-685.34018	48.5
^{5}TS4-1	-0.02483	-685.35083	20.5
^{3}TS4-2	-0.02770	-685.34123	45.8
^{5}TS4-2	-0.02957	-685.34281	41.6
$^3NRh_4^+OCO$	-0.02886	-685.35849	0.4
$^5NRh_4^+OCO$	-0.02913	-685.35684	4.8
^{3}TS4-3	-0.02820	-685.35708	4.1
^{5}TS4-3	-0.02978	-685.35558	8.1
$^3NRh_4^+O_bCO$	-0.02620	-685.39866	-105.0
$^5NRh_4^+O_bCO$	-0.02886	-685.39449	-94.1
^{3}TS4-4	-0.02671	-685.36084	-5.7
^{5}TS4-4	-0.02670	-685.36363	-13.1
$^3NRh_4^+CO_2$	-0.02980	-685.40898	-132.1
$^5NRh_4^+CO_2$	-0.03115	-685.42223	-166.9
CO_2	-0.00969	-188.66033	

$^{3}NRh_4^+$	-0.03312	-496.74648	
$^{3}NRh_4^+ + CO_2$	-0.04281	-685.40681	-126.4
$^{5}NRh_4^+$	-0.03493	-496.76090	
$^{5}NRh_4^+ + CO_2$	-0.04462	-685.42123	-164.3
$^{7}NRh_4^+$	-0.03620	-496.74820	
^{3}TS4-4	-0.03350	-496.73670	
^{3}TS4-4 + CO_2	-0.04319	-685.39703	-100.7
^{5}TS4-4	-0.03441	-496.75064	
^{5}TS4-4 + CO_2	-0.04410	-685.41097	-137.3
$^{3}N_bRh_4^+$	-0.03114	-496.80242	
$^{3}N_bRh_4^+ + CO_2$	-0.04083	-685.46275	-273.3
$^{5}N_bRh_4^+$	-0.03228	-496.81464	
$^{5}N_bRh_4^+ + CO_2$	-0.04197	-685.47497	-305.4
$^{7}N_bRh_4^+$	-0.03321	-496.79666	

Table S5: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^4Rh_4^+$ + 2NO + CO for all the species plus CO_2 in the reaction of $N_bRh_4^+$ + NO → Rh_4^+ + N_2O at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
NO	-0.01553	-129.94980	
$^3N_bRh_4^+$	-0.03114	-496.80242	
$^3N_bRh_4^+$ + NO	-0.04668	-626.75222	32.1
$^5N_bRh_4^+$	-0.03228	-496.81464	
$^5N_bRh_4^+$ + NO	-0.04781	-626.76444	0.0
$^4N_bRh_4^+(NO)_b$	-0.02717	-626.80318	-101.7
$^6N_bRh_4^+(NO)_b$	-0.02777	-626.78628	-57.3
$^2N_bRh_4^+(NO)$	-0.02820	-626.80446	
$^4N_bRh_4^+(NO)$	-0.02843	-626.81187	-124.5
$^6N_bRh_4^+(NO)$	-0.02983	-626.79617	-83.3
^{2}TS5-1	-0.02934	-626.73913	
^{4}TS5-1	-0.03015	-626.75158	33.8
^{6}TS5-1	-0.03096	-626.74656	46.9
$^2NRh_4^+NO$	-0.02847	-626.75029	
$^4NRh_4^+NO$	-0.03044	-626.76038	10.7
$^6NRh_4^+NO$	-0.03211	-626.74935	39.6
^{2}TS5-2	-0.03001	-626.71366	
^{4}TS5-2	-0.03000	-626.72403	106.1
^{6}TS5-2	-0.03185	-626.71981	117.2
$^4Rh_4^+N_2O$	-0.02565	-626.75979	40.7
$^6Rh_4^+N_2O$	-0.02702	-626.76329	5.9
N_2O	-0.01024	-184.73455	
$^4Rh_4^+$ + N_2O	-0.04548	-626.77731	-33.8
$^6Rh_4^+$ + N_2O	-0.04593	-626.77629	-31.1
^{4}TS5-3	-0.02940	-626.69752	175.7
^{6}TS5-3	-0.02957	-626.68447	210.0

$^4(N)_b(N)Rh_4^+O$	-0.02971	-626.72286	109.2
$^6(N)_b(N)Rh_4^+O$	-0.03183	-626.70538	155.1
^{4}TS5-4	-0.03309	-626.64069	324.9
^{6}TS5-4	-0.03212	-626.63130	349.6
$^4(N)_2Rh_4^+O$	-0.03326	-626.64145	322.9
$^6(N)_2Rh_4^+O$	-0.03415	-626.63900	329.4

Table S6: Thermal correction to Gibbs free energy (G_0) (hartree), sum of electronic and thermal free energies (G_c) (hartree) corrected by G_0, relative free energies (G_r) (kJ mol^{-1}) to $^4Rh_4^+$ + NO + 2CO for all the species plus CO_2 in the two reactions of $N_bRh_4^+$ + CO → Rh_4^+ + NCO and Rh_4^+ + NCO → $O_bRh_4^+$ + CN at the B3LYP/6-311+G(2d), SDD level in the gas phase under atmospheric pressure and room temperature (300 K and 1 atm).

Species	B3LYP/6-311+G(2d), SDD in the gas phase (300 K and 1 atm)		
	G_0	G_c	G_r
CO	-0.01408	-113.36610	
$^3N_bRh_4^+$	-0.03114	-496.80242	
$^3N_bRh_4^+$ + CO	-0.04523	-610.16852	32.1
$^5N_bRh_4^+$	-0.03228	-496.81464	
$^5N_bRh_4^+$ + CO	-0.04636	-610.18073	0.0
$^1N_bRh_4^+CO$	-0.02543	-610.16122	
$^3N_bRh_4^+CO$	-0.02665	-610.20953	-75.6
$^5N_bRh_4^+CO$	-0.02866	-610.20702	-69.0
^{1}TS6-1	-0.02737	-610.14894	
^{3}TS6-1	-0.02883	-610.14862	84.3
^{5}TS6-1	-0.02868	-610.15605	64.8
$^3Rh_4^+N_bCO$	-0.02524	-610.17190	23.2
$^5Rh_4^+N_bCO$	-0.02544	-610.18319	-6.4
$^7Rh_4^+N_bCO$	-0.02858	-610.18319	
NCO	-0.00724	-168.06512	
$^4Rh_4^+$ + NCO	-0.04248	-610.10788	191.3
$^6Rh_4^+$ + NCO	-0.04293	-610.10686	193.9
$^1Rh_4^+NCO$	-0.02566	-610.16404	
$^3Rh_4^+NCO$	-0.02683	-610.16416	43.5
$^5Rh_4^+NCO$	-0.02821	-610.17139	24.5
^{3}TS6-2	-0.02819	-610.08454	252.5
^{5}TS6-2	-0.02914	-610.08752	244.7
$^1O_bRh_4^+CN$	-0.02635	-610.13183	
$^3O_bRh_4^+CN$	-0.02722	-610.13168	128.8
$^5O_bRh_4^+CN$	-0.02869	-610.13100	130.6
CN	-0.01478	-92.75579	

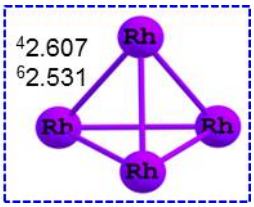
$^{4}O_bRh_4^+$ + CN	-0.04735	-610.03460	383.7
$^{6}O_bRh_4^+$ + CN	-0.04928	-610.04518	355.9

Table S7: Snapshot and standard orientation of all the species in the gas phase calculated at the B3LYP/6-311+G(2d), SDD level. Distance lengths are reported in Å.

NO

N	0.00000000	0.00000000	-0.61196800
O	0.00000000	0.00000000	0.53547200

Rh_4^+



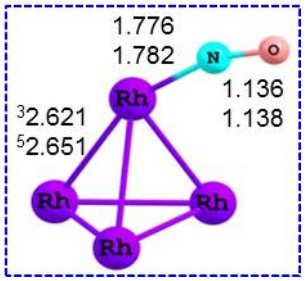
$^4Rh_4^+$

Rh	0.78744900	-0.40584000	1.26393300
Rh	-1.42188400	-0.78236500	-0.06874200
Rh	0.91480200	-0.38464700	-1.19490900
Rh	-0.28036800	1.57285300	-0.00028300

$^6Rh_4^+$

Rh	-0.30961600	-1.12122300	1.02455600
Rh	1.20467800	-0.47484200	-0.91002500
Rh	0.44222400	1.32580300	0.70825500
Rh	-1.33728600	0.27026200	-0.82278500

Rh_4^+NO



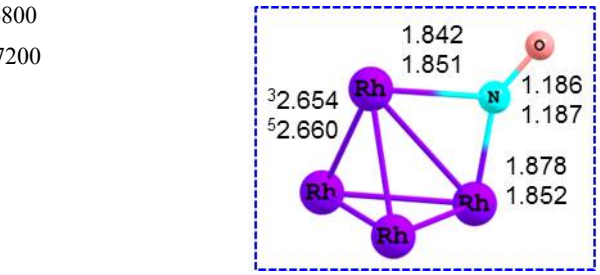
$^3Rh_4^+NO$

Rh	1.08633600	-0.41259800	-0.81336100
Rh	-1.50461500	-0.03437200	-0.92877400
Rh	-0.02003700	1.48465200	0.51793300
Rh	-0.63554700	-0.97371800	1.16600100
N	2.74207900	-0.28824400	-0.18335600
O	3.64115500	-0.10758900	0.48781800

$^5Rh_4^+NO$

Rh	-1.08923300	-0.93039600	-0.06971100
Rh	1.54928200	-0.89788600	-0.32327200
Rh	0.48877700	0.62901700	1.40817300
Rh	0.13124400	1.18873400	-1.05104000
N	-2.76868900	-0.34418700	0.04013200
O	-3.65279400	0.36040200	0.16653800

b-Rh_4^+NO



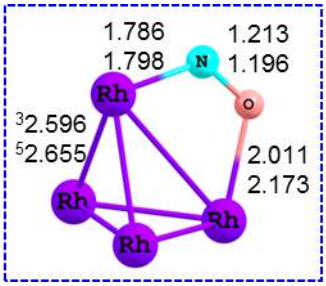
^{3}b-Rh_4^+NO

Rh	-0.99494600	-1.34978700	0.00035700
Rh	1.06800100	-0.18708000	-1.19829600
Rh	1.06617300	-0.18509800	1.19932700
Rh	-0.34762500	1.56380200	-0.00094400
N	-1.75996400	0.32618800	-0.00097700
O	-2.91280000	0.60425200	-0.00164300

^{5}b-Rh_4^+NO

Rh	0.72685400	1.49392500	0.00007300
Rh	-1.13624800	0.00002400	-1.17246000
Rh	-1.13603700	-0.00029400	1.17258400
Rh	0.72727400	-1.49371400	-0.00017600
N	1.82119500	0.00006600	-0.00017600
O	3.00859100	0.00027700	0.00003500

bb-Rh_4^+NO



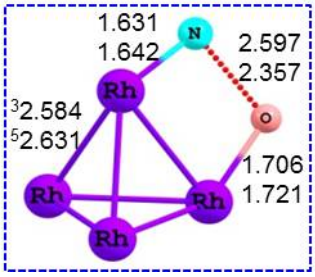
^{3}bb-Rh_4^+NO

Rh	1.72789900	0.25783800	-0.09306000
Rh	-0.23291900	-0.87961500	1.28426300
Rh	-0.28745900	-1.04838300	-1.12928000
Rh	-1.40342200	0.95208600	-0.08595100
N	1.19858000	1.94319600	0.07522700
O	0.05318700	2.33887200	0.06933000

^{5}bb-Rh_4^+NO

Rh	-0.79057000	1.33505800	-0.03346800
Rh	0.66501100	-0.29254100	1.47624500
Rh	1.47452600	0.30636900	-0.88562300
Rh	-0.52565700	-1.31114900	-0.55601700
N	-2.38291800	0.51042500	0.09951300
O	-2.54606900	-0.65889500	-0.09347400

TS1-1



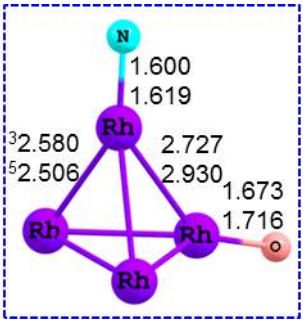
^{3}TS1-1 (-84.2 i)

Rh	-0.18278900	0.27162400	0.01344700
Rh	-0.11760200	-0.14570500	2.56261200
Rh	2.06438700	-0.13310400	1.16690000
Rh	0.93735900	-2.32067700	1.69505500
N	-0.76273300	-0.91806000	-0.93917800
O	0.08064100	-2.99042900	0.37993000

^{5}TS1-1 (-108.1 i)

Rh	1.76280600	-0.43357100	-0.22616700
Rh	-0.00354900	1.47950400	-0.60135800
Rh	-0.04803900	-0.02537700	1.52997000
Rh	-1.73758000	-0.47963500	-0.26911200
N	1.33054700	-1.68383300	-1.19939800
O	-1.01594000	-1.56932700	-1.38801900

NRh_4^+O



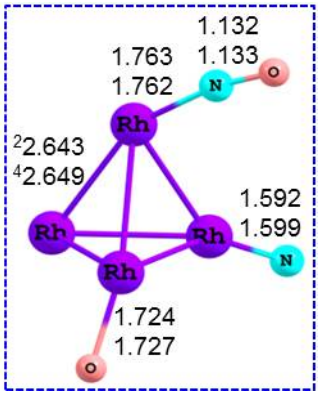
^{3}NRh_4^+O

Rh	1.43369400	0.67243200	-0.00099500
Rh	-0.04954700	-0.97514100	1.31905100
Rh	-0.04853500	-0.98243800	-1.31418900
Rh	-1.29271400	0.72391400	-0.00242100
N	2.72168700	1.62112700	-0.00472000
O	-2.62278100	1.73844600	-0.00400000

^{5}NRh_4^+O

Rh	1.56379600	-0.00113900	0.45403500
Rh	-0.11184800	-1.31774700	-0.86434700
Rh	-0.11209200	1.32432900	-0.85515000
Rh	-1.30711200	-0.00470000	1.04092400
N	2.99796900	-0.00596800	1.20526600
O	-2.80740800	0.00104400	0.20842000

NRh_4^+O(NO)



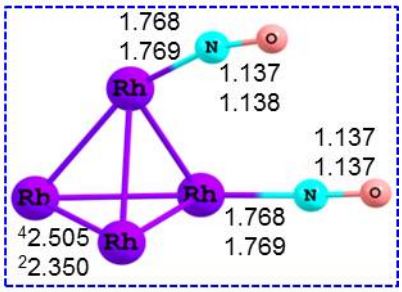
^{2}NRh_4^+O(NO)

Rh	1.29795300	-0.37706800	0.81843600
Rh	-1.24762300	0.14859100	1.29567500
Rh	-0.69498100	-1.16786900	-0.87429700
Rh	-0.01406400	1.37795500	-0.57692500
N	2.75220200	-0.56497900	-0.16055500
O	-2.29535800	-1.23330300	-1.51171400
O	3.56041700	-0.62378100	-0.95160200
N	0.03661100	2.80559200	-1.28565700

^{4}NRh_4^+O(NO)

Rh	1.29937900	-0.42298900	0.79966900
Rh	-1.25970900	0.07349700	1.27065200
Rh	-0.67538600	-1.12157200	-0.92851700
Rh	-0.02333200	1.41877200	-0.49956400
N	2.76342900	-0.53651400	-0.17332800
O	-2.30522000	-1.20079600	-1.49276500
O	3.57741200	-0.55400000	-0.96066100
N	0.01937700	2.87816200	-1.15144200

$ONRh_4^+NO$



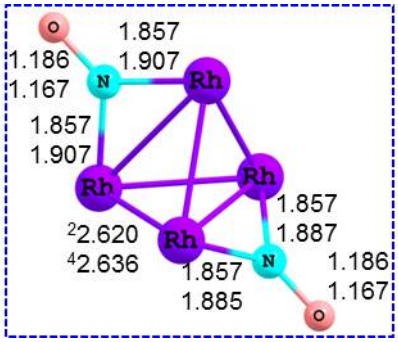
$^2ONRh_4^+NO$

Rh	-0.32951400	-1.34468200	-0.60814900
Rh	1.90903300	-0.00250000	-0.41597900
Rh	0.38545900	-0.00530000	1.57234200
Rh	-0.32285500	1.35125900	-0.60043300
N	-1.91757700	-1.98401000	-0.16667100
O	-2.94209000	2.15647000	0.28965400
O	-2.94419400	-2.15492100	0.29129800
N	-1.91174600	1.99009900	-0.16158100

$^4ONRh_4^+NO$

Rh	-0.42282000	-1.33978900	-0.56796800
Rh	1.87456200	0.00468800	-0.53176600
Rh	0.68027900	-0.01039200	1.49173000
Rh	-0.42243500	1.34907900	-0.54885600
N	-2.02552700	-1.88150600	-0.05047000
O	-3.04238800	1.96250400	0.47542300
O	-3.02343300	-1.97951600	0.48667900
N	-2.03229800	1.87789800	-0.04068400

$(NO)_bRh_4^+(NO)_b$



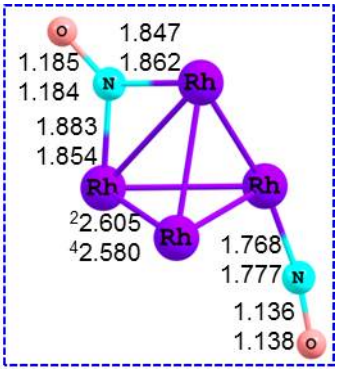
$^2(NO)_bRh_4^+(NO)_b$

Rh	0.80409600	-0.82356500	-1.20781500
Rh	0.80705500	0.82159800	1.20741200
Rh	-0.80667900	-1.20674100	0.82323500
Rh	-0.80462000	1.20859300	-0.82185700
N	1.95196600	-0.00104800	-0.00116000
O	-3.13737500	0.00132600	-0.00175100
O	3.13780000	-0.00077900	-0.00222100
N	-1.95150800	0.00116000	-0.00055900

$^4(NO)_bRh_4^+(NO)_b$

Rh	0.84594700	-0.00472300	-1.31564200
Rh	0.84268600	-0.00556900	1.31687900
Rh	-0.88502200	-1.49940700	-0.00131300
Rh	-0.86968600	1.50443400	-0.00056700
N	2.22428000	0.00123500	0.00184800
O	-3.19974300	0.01678700	0.00085700
O	3.39109700	0.00353700	0.00192600
N	-2.01820000	0.00938400	-0.00089200

$ONRh_4^+(NO)_b$



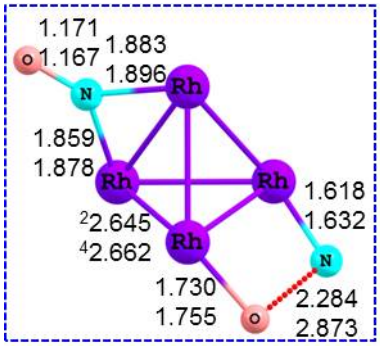
$^2ONRh_4^+(NO)_b$

Rh	-1.14163900	-0.36923500	-0.85627200
Rh	-0.12451800	-0.47289200	1.56075600
Rh	0.35055600	1.62995100	0.09910300
Rh	1.25975300	-1.16208600	-0.44009800
N	-2.81012700	0.13780900	-0.56565200
O	2.81814600	1.06684700	-0.91725900
O	-3.84510400	0.35167600	-0.14813300
N	1.77139100	0.64699900	-0.55347400

$^4ONRh_4^+(NO)_b$

Rh	-1.13905000	-0.45196000	-0.85634800
Rh	-0.23319100	-0.26944000	1.60929100
Rh	0.40344400	1.60328800	-0.04652000
Rh	1.29253100	-1.21175600	-0.29404100
N	-2.82900300	0.06821100	-0.68455600
O	2.87522600	0.93963400	-0.97699300
O	-3.82654900	0.38533200	-0.23787700
N	1.83508100	0.53812700	-0.57804900

TS1-2



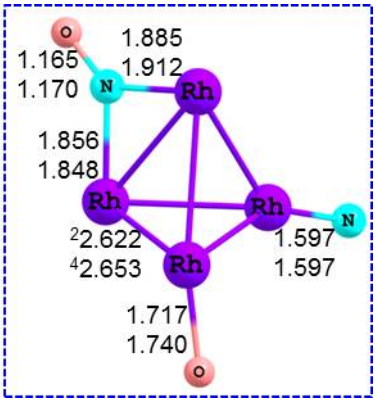
^{2}TS1-2 (-152.4 i)

Rh	0.97157500	0.20938300	-1.31263200
Rh	0.78533400	-0.29412700	1.36437700
Rh	-0.98923000	-1.32335400	-0.30477500
Rh	-0.84179500	1.40180200	0.17650200
N	2.15527500	-0.07901400	0.09107400
O	-2.65401800	-1.24117100	0.04584100
O	3.32407500	-0.07390700	0.17018800
N	-2.44459900	1.62243700	0.15400200

^{4}TS1-2 (-168.3 i)

Rh	-1.03551100	-0.71444200	-1.10015700
Rh	-0.80045500	0.41041600	1.33415700
Rh	0.74848000	1.22773000	-0.67030200
Rh	1.16702100	-1.14938900	0.36575000
N	-2.20914300	0.13160200	0.09662200
O	2.42663700	1.41828000	-0.19262000
O	-3.34586800	0.39368000	0.11706700
N	2.74839700	-0.75157700	0.44327200

$NRh_4^+O(NO)_b$



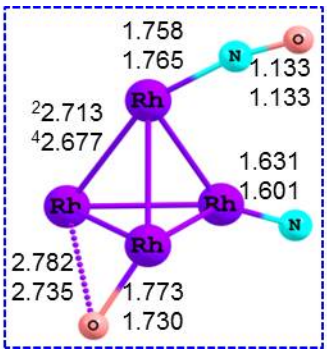
$^{2}NRh_4^+O(NO)_b$

Rh	1.09865200	0.21236900	-1.23531700
Rh	0.65699000	-0.62458000	1.25165400
Rh	-1.26306100	-1.06212400	-0.47895200
Rh	-0.70281200	1.37075200	0.26691400
N	2.19974200	-0.26967600	0.17903900
O	-2.85344000	-1.32631600	0.11230800
O	3.34730200	-0.28712800	0.38066300
N	-1.41267300	2.77950300	0.51563900

$^{4}NRh_4^+O(NO)_b$

Rh	-1.15873900	0.31362400	1.22018300
Rh	-0.58249300	-0.80018500	-1.21335800
Rh	1.32657600	-0.94180200	0.62363000
Rh	0.62896600	1.35042300	-0.36947000
N	-2.11573800	-0.37567000	-0.20291600
O	2.87028200	-1.19723400	-0.13773200
O	-3.25438600	-0.47416700	-0.45303500
N	1.17700700	2.78688300	-0.79968300

TS1-3



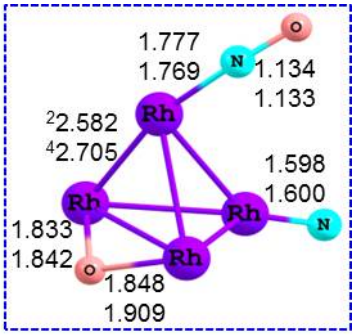
^{2}TS1-3 (-162.3 i)

Rh	1.22098300	-0.62138200	0.76516000
Rh	-1.34990700	-0.00955100	1.18344400
Rh	-0.60519400	-0.97528800	-1.13563100
Rh	0.03841600	1.45924000	-0.33598500
N	2.79394500	-0.50365200	-0.03503900
O	-2.32902500	-1.04953900	-1.19097900
O	3.66824700	-0.28294100	-0.71991000
N	0.14789000	2.97136300	-0.84744400

^{4}TS1-3 (-222.1 i)

Rh	1.24387900	-0.61298700	0.74701700
Rh	-1.33396700	-0.03409000	1.19400500
Rh	-0.61843100	-0.98507300	-1.13667700
Rh	0.01569200	1.45831500	-0.32776500
N	2.80853100	-0.47100900	-0.05773500
O	-2.34828000	-0.96375500	-1.17225200
O	3.68718900	-0.25169900	-0.73785300
N	0.11517300	2.97760800	-0.82301000

$NRh_4^+O_b(NO)$



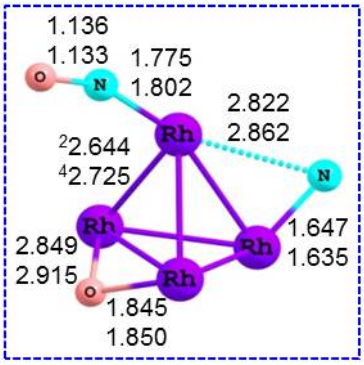
$^{2}NRh_{4}^{+}O_{b}(NO)$

Rh	-1.08872700	-0.79312200	-0.54250200
Rh	1.48462300	-0.92158100	-0.71607600
Rh	-0.10683200	0.00759700	1.74251100
Rh	0.46003400	1.38752600	-0.35387600
N	-2.75491300	-0.17870300	-0.49374000
O	1.29956100	-1.00785500	1.10583100
O	-3.69515200	0.42848400	-0.67351500
N	0.67710500	2.89528600	-0.83641500

$^{4}NRh_{4}^{+}O_{b}(NO)$

Rh	-1.16354600	-0.73392700	-0.67751200
Rh	1.47821600	-0.32094600	-1.08735600
Rh	0.38440400	-0.71265400	1.50466800
Rh	0.06576900	1.46021000	0.13152100
N	-2.83699800	-0.37337000	-0.23320800
O	2.07243800	-0.70101800	0.61396800
O	-3.80271500	0.08807700	0.13898400
N	-0.10239100	3.04947900	0.19990700

TS1-4



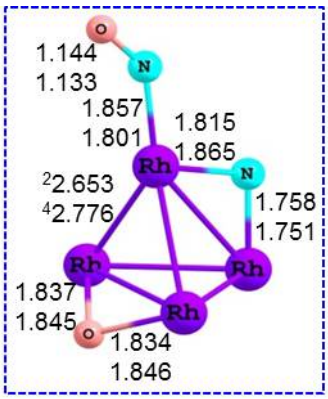
^{2}TS1-4 (-98.7 i)

Rh	1.69414900	-0.01174900	0.41743000
Rh	0.02314200	1.50344900	-0.79349300
Rh	-0.96638700	-0.00210800	1.08806100
Rh	0.00384800	-1.48945500	-0.81401200
N	2.17074300	-0.02398100	1.98040300
O	-0.15217400	0.01553300	-1.87312200
N	-2.72062700	0.00235300	0.75688900
O	-3.61215200	0.00261900	0.05182800

^{4}TS1-4 (-175.4 i)

Rh	1.58874400	-0.04404400	0.64401700
Rh	0.14132200	1.64085300	-0.63339800
Rh	-1.07309700	-0.12949200	0.92910900
Rh	0.20340800	-1.40835900	-1.03015400
N	1.45546400	-0.49184400	2.22834700
O	0.10570900	0.25797100	-1.85437400
N	-2.79660300	-0.09674100	0.52946700
O	-3.77183300	-0.07460100	-0.05006500

$N_{b}Rh_{4}^{+}O_{b}(NO)$



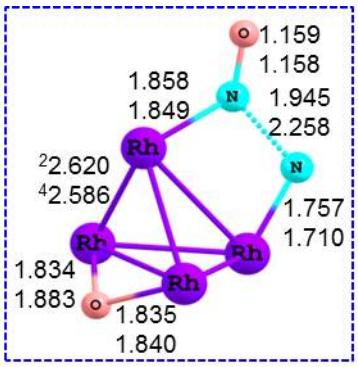
$^{2}N_{b}Rh_{4}^{+}O_{b}(NO)$

Rh	-1.37662200	-0.02891000	0.12071100
Rh	0.63799200	1.47577300	-0.72525100
Rh	0.69957700	-1.45589400	-0.73421700
Rh	1.16970900	0.01296500	1.37260500
N	-3.22111300	-0.02821200	0.33493300
O	1.13145800	0.02142300	-1.73240900
O	-4.19146600	-0.00266200	-0.27101400
N	-0.55024100	-0.01851800	1.73709800

$^{4}N_{b}Rh_{4}^{+}O_{b}(NO)$

Rh	1.41846800	0.05551700	0.07494700
Rh	-0.88463100	1.45664600	-0.58803300
Rh	-0.91841800	-0.50200800	1.47560600
Rh	-0.69783800	-1.10523400	-1.05296600
N	3.20593100	0.21862600	0.22657100
O	-1.89713500	0.93958500	0.86485300
O	4.26998100	0.51499200	0.47931500
N	1.04065800	-1.26977900	-1.18132600

TS1-5



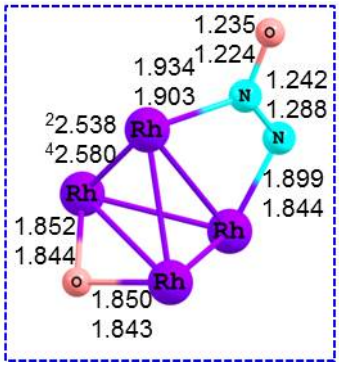
^{2}TS1-5 (-123.9 i)

Rh	1.45876900	-0.72803100	-0.00132200
Rh	-0.68560300	-0.60800200	1.48538500
Rh	-0.68905100	-0.61015400	-1.48318900
Rh	-0.85658900	1.48946300	-0.00036700
N	2.21764300	0.96960800	-0.00248100
O	-1.40062900	-1.43437600	0.00250700
O	3.37537100	1.04024500	-0.00045800
N	0.49141100	2.41690600	-0.00312400

^{4}TS1-5 (-208.3 i)

Rh	-1.62523300	-0.43910100	-0.06626200
Rh	0.59909000	-1.08362600	-1.18820600
Rh	0.36825200	-0.27779600	1.63256100
Rh	1.31944400	1.21279900	-0.26515500
N	-2.04021400	1.29747400	-0.58762200
O	0.93796400	-1.64746900	0.54716600
O	-3.02403800	1.74667500	-0.16802400
N	0.17145600	2.36738000	-0.57171300

$ON_2Rh_4^+O_b$



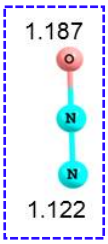
$^{2}ON_2Rh_4^+O_b$

Rh	1.24313800	-0.97085000	0.00567400
Rh	-0.75888000	-0.44426000	1.47482400
Rh	-0.77222800	-0.48075100	-1.45867300
Rh	-0.52361700	1.57808100	-0.01686600
N	2.05147500	0.78613800	-0.01447900
O	-1.69445100	-1.10410300	0.01921600
O	3.27442700	0.61258600	-0.01281500
N	1.36017700	1.81846800	-0.02471400

$^{4}ON_2Rh_4^+O_b$

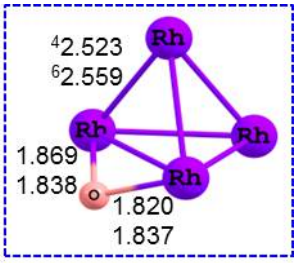
Rh	1.18295600	-1.06963300	0.01065100
Rh	-0.82624400	-0.39048700	1.47927900
Rh	-0.83543500	-0.43290600	-1.46467600
Rh	-0.35870800	1.62950000	-0.02095500
N	2.12437800	0.58441000	-0.01154100
O	-1.78780300	-0.97309000	0.01728300
O	3.34140600	0.45538300	-0.01190700
N	1.48356100	1.70134500	-0.02224100

N_2O



N	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.12179400
O	0.00000000	0.00000000	2.30904500

$O_bRh_4^+$



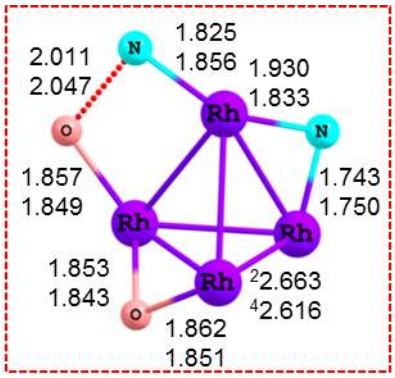
$^{4}O_bRh_4^+$

Rh	1.42819100	0.11547300	-0.68941300
Rh	-0.60417200	1.47885900	-1.30076200
Rh	0.09810300	0.63676000	1.52153000
Rh	-0.74040300	-0.89263800	-0.45301900
O	-0.63443900	1.95816300	0.50597500

$^{6}O_bRh_4^+$

Rh	1.47793700	0.15905100	-0.69800600
Rh	-0.59434500	1.52950700	-1.30968200
Rh	0.08099800	0.59184500	1.49181200
Rh	-0.78781700	-0.93426900	-0.37943100
O	-0.62949400	1.95048300	0.47961800

TS1-6



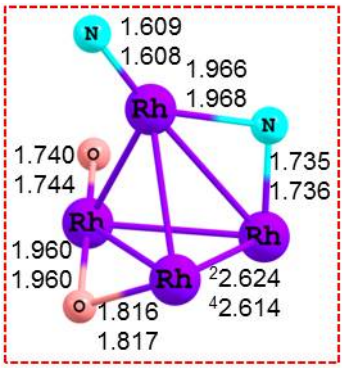
^{2}TS1-6 (-94.5 i)

Rh	0.80135700	-1.24557100	0.65987600
Rh	0.87155300	1.18682800	-0.58066300
Rh	-1.11747700	0.60339300	1.20701300
Rh	-1.22392900	-0.56914600	-1.20221700
N	2.42817800	-1.15683400	0.50253300
O	-0.40757700	2.10768800	0.35412600
O	2.52339100	0.80139200	-0.79287900
N	-0.54877800	-2.01035800	-0.54115500

^{4}TS1-6 (-254.8 i)

Rh	1.45521300	0.19871300	0.05600700
Rh	-0.86195600	1.60262200	-0.47011600
Rh	-0.81259600	-0.50754300	1.50679700
Rh	-0.75241900	-1.04438400	-1.10127400
N	2.31049700	1.61902800	-0.18978100
O	-1.94630300	0.79995700	0.80637400
O	0.17714300	2.86702300	-0.95224600
N	0.98425700	-1.21716300	-1.15082400

$(N)_2Rh_4^+(O)_2$



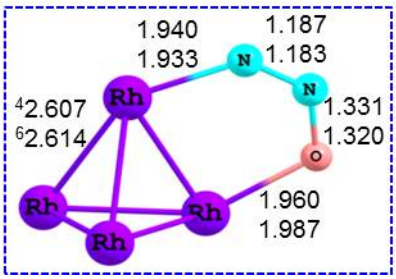
$^{2}(N)_2Rh_4^+(O)_2$

Rh	-0.46622200	1.43596700	0.44913900
Rh	1.45058600	0.03160600	-0.78891700
Rh	-1.51673500	-0.64697600	-0.76988000
Rh	0.19567100	-1.30986200	1.10435500
N	-0.85192600	2.97502900	0.18245800
O	-0.07183500	-0.56679800	-1.86780300
O	2.87632800	0.56831600	0.05254100
N	-0.18871100	0.16851000	1.92621400

$^{4}(N)_2Rh_4^+(O)_2$

Rh	-0.45607300	1.44321000	0.44027100
Rh	1.43588300	0.02900200	-0.81123300
Rh	-1.50748900	-0.66112300	-0.75901400
Rh	0.19649900	-1.29068300	1.12122000
N	-0.82375100	2.98256200	0.15693800
O	-0.08541400	-0.57863300	-1.88674700
O	2.84355800	0.50016200	0.10412200
N	-0.19939700	0.19022200	1.93663900

$Rh_4^+ON_2$



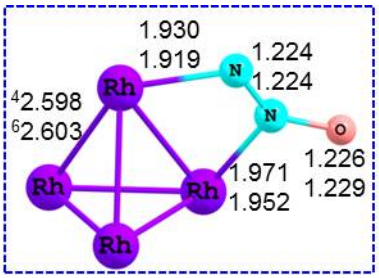
$^{4}Rh_4^+ON_2$

Rh	-1.49723800	0.03639100	-1.01285200
Rh	0.58547600	-1.18931200	-0.14432100
Rh	-0.92781900	-0.20304600	1.50320800
Rh	0.51467200	1.31823900	0.03955700
N	2.44105700	1.10807200	-0.05476400
N	3.06749800	0.10423000	-0.14508100
O	2.54329100	-1.11822000	-0.18814500

$^{6}Rh_4^+ON_2$

Rh	1.53743700	0.22462200	-0.97758000
Rh	-0.57978600	1.25520400	-0.05195500
Rh	0.90637400	-0.25234400	1.46551100
Rh	-0.55682100	-1.25749500	-0.47871300
N	-2.43987000	-1.05397400	-0.09170000
N	-3.04998200	-0.06931300	0.14766600
O	-2.54940400	1.15169700	0.19142200

$Rh_4^+N_2O$



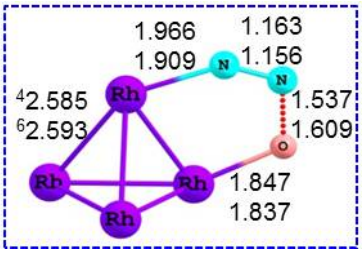
$^{4}Rh_4^+N_2O$

Rh	-1.46467400	-0.53856000	-0.93311200
Rh	0.84326200	-1.15602800	-0.00414100
Rh	-0.90686600	0.20984800	1.45951700
Rh	0.22727400	1.39253900	-0.53454800
N	2.12443600	1.24234600	-0.21371700
N	2.38875700	0.06730200	0.00593100
O	3.36910500	-0.62731100	0.25091300

$^{6}Rh_4^{+}N_2O$

Rh	-1.47208700	-0.54792200	-0.86414500
Rh	0.85785300	-1.18244700	-0.09482600
Rh	-0.83428200	0.18025200	1.47705900
Rh	0.18089800	1.43938900	-0.55590200
N	2.04207700	1.28312700	-0.11515400
N	2.32268000	0.10117000	0.03804200
O	3.31118800	-0.58841100	0.28018100

TS2-1



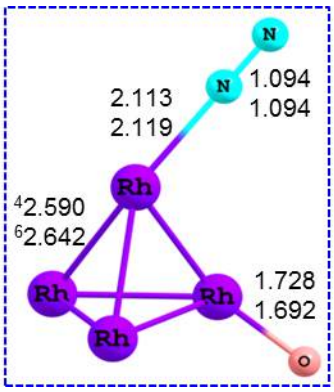
^{4}TS2-1 (-611.6 i)

Rh	-0.20881100	-0.11756700	0.13756200
Rh	0.28004300	0.14807400	2.59590100
Rh	2.22160000	0.16906400	0.98179200
Rh	0.95856700	-2.04865800	1.39856400
N	0.42946200	-2.78021100	3.14547100
N	0.02762800	-2.30332400	4.12676200
O	-0.15586600	-0.77720500	4.13328600

^{6}TS2-1 (-573.4 i)

Rh	-0.35667100	-0.37136900	0.34702400
Rh	0.55650200	0.16405800	2.68381100
Rh	2.18807500	0.34887200	0.81564700
Rh	1.23399100	-2.04211900	1.53040800
N	0.27662900	-2.74371000	3.02611400
N	-0.24130900	-2.32961800	3.97332800
O	-0.10459500	-0.73594100	4.14300600

$ORh_4^{+}N_2$



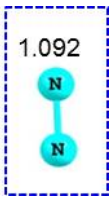
$^{4}ORh_4^{+}N_2$

Rh	1.75412000	-0.23513500	-0.74244000
Rh	-0.26381200	1.54969600	-0.48552000
Rh	0.61311400	0.18026400	1.41872600
Rh	-0.71646300	-0.96641400	-0.47548600
N	-2.75141000	-1.29128100	-0.00624600
N	-3.80922600	-1.41877400	0.24362300
O	-1.72220100	2.31438600	0.03836700

$^{6}ORh_4^{+}N_2$

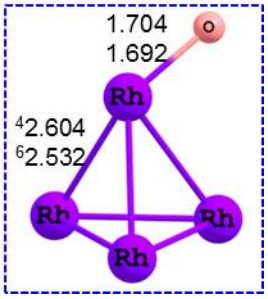
Rh	1.37223700	-0.05821000	-0.99488500
Rh	-0.62451400	1.36737500	-0.43240600
Rh	0.91314900	0.36193400	1.45208400
Rh	-0.77631400	-1.08814800	0.14750400
N	-2.82948700	-1.56884900	-0.06194300
N	-3.89081100	-1.80830500	-0.17694600
O	-1.06013900	2.92694400	0.05761500

N_2



N	0.00000000	0.00000000	0.54580000
N	0.00000000	0.00000000	-0.54580000

ORh_4^{+}



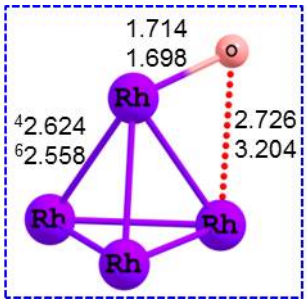
$^{4}ORh_4^{+}$

Rh	1.58394500	-0.01399800	-0.75474000
Rh	-0.56639200	1.45409300	-0.81739300
Rh	0.31972600	0.22680400	1.43935000
Rh	-0.72114800	-1.11803000	-0.45378700
O	-1.06885100	2.74774900	0.17088200

$^{6}ORh_4^{+}$

Rh	1.42582000	0.27464100	-0.83415300
Rh	-0.80340100	1.36075700	0.04173700
Rh	0.54679100	-0.18508900	1.51967000
Rh	-0.71658800	-1.09212100	-0.58091700
O	-0.90534100	2.93843000	-0.56202400

TS2-2



^{4}TS2-2 (-100.0 i)

Rh	0.25596700	0.41308900	0.09075500
Rh	0.17489900	0.03095800	2.79187200
Rh	2.36500700	-0.25041800	1.50451600
Rh	0.47987700	-1.95154400	1.20898100
O	-0.85055500	1.53595700	0.76397200

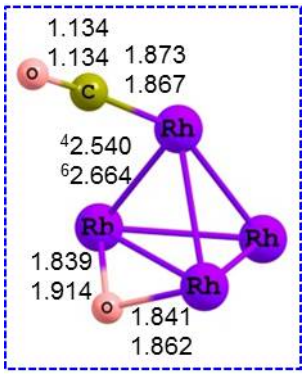
^{6}TS2-2 (-98.4 i)

Rh	0.22258200	0.40105800	0.23540300
Rh	0.26877200	-0.11391000	2.92882600
Rh	2.36626800	-0.20919700	1.49079000
Rh	0.45821400	-1.95143000	1.18539300
O	-0.89064100	1.65152000	0.51968500

CO

O	0.00000000	0.00000000	0.48243300
C	0.00000000	0.00000000	-0.64324400

$O_bRh_4^{+}CO$



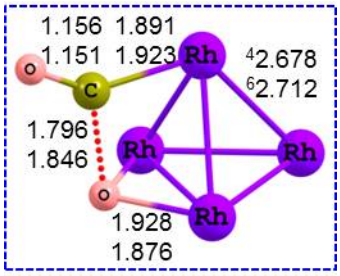
$^{4}O_bRh_4^{+}CO$

Rh	1.17662000	0.45132000	-0.54043000
Rh	-1.10578500	1.26585900	-1.36928400
Rh	-0.47891700	0.41515100	1.43470400
Rh	-0.93154100	-1.17431000	-0.49452500
O	-1.34062500	1.67578700	0.40990900
O	-3.79613800	-1.87782600	0.08285700
C	-2.70836200	-1.65619800	-0.14959200

$^{6}O_bRh_4^{+}CO$

Rh	1.29492700	0.31704500	-0.62613100
Rh	-1.08551200	1.19300600	-1.20204000
Rh	-0.36151300	0.57394100	1.35676600
Rh	-0.87879400	-1.25744400	-0.50741500
O	-1.68775100	1.65477200	0.49806600
O	-3.78418700	-1.76801700	0.03548000
C	-2.68191800	-1.61352100	-0.18108600

TS3-1



^{4}TS3-1(-362.2 i)

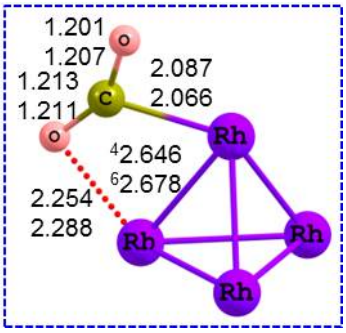
Rh	1.02278200	0.47757300	-0.49431400
Rh	-1.19783600	1.13212300	-1.45722200
Rh	-0.48824900	0.24363600	1.49310000
Rh	-0.91975800	-1.36418400	-0.57646700
O	-1.78486100	1.13431500	0.37944000
O	-3.60745000	-0.62379500	0.24022300
C	-2.47929400	-0.48483400	0.03250400

^{6}TS3-1 (-451.4 i)

Rh	0.98599800	0.39435700	-0.44646900
Rh	-0.94324900	1.27337000	-1.55118800
Rh	-0.77373600	0.17739800	1.43848000

Rh	-0.94978700	-1.35808200	-0.73618200
O	-1.87312700	1.24518700	0.24668700
O	-3.50687000	-0.73428100	0.44359100
C	-2.39389300	-0.48311600	0.22234400

$Rh_4^+CO_2$



$^4Rh_4^+CO_2$

Rh	0.17931100	1.46446000	0.28926100
Rh	-1.54535800	-0.07060000	-1.08814900
Rh	-0.85872900	-0.62234900	1.43086300
Rh	0.83449900	-0.99887100	-0.42138100
O	2.42991400	1.38408500	0.19284900
C	2.50540800	0.20662600	-0.09027600
O	3.16352200	-0.77119700	-0.32106500

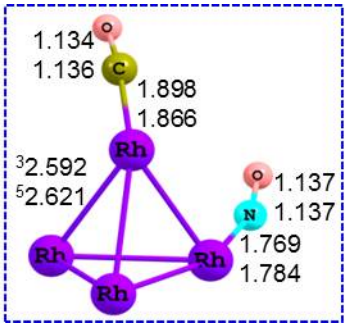
$^6Rh_4^+CO_2$

Rh	0.14995500	1.45759300	0.20737000
Rh	-1.50141100	-0.06263400	-0.98824000
Rh	-0.92400000	-0.59748400	1.43079500
Rh	0.89157600	-1.02615000	-0.46591100
O	2.43637600	1.37387500	0.24980000
C	2.50064900	0.21054300	-0.08006400
O	3.15542100	-0.76358900	-0.36164900

CO_2

O	-0.96225400	1.03839700	0.00118200
C	-2.12197500	1.07508200	-0.00316000
O	-3.28169700	1.11176800	-0.00750200

$ONRh_4^+CO$



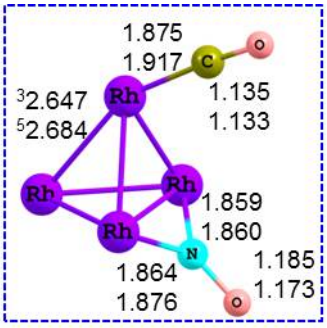
$^3ONRh_4^+CO$

Rh	0.24274900	1.48721500	-0.30824900
Rh	-1.95118200	-0.06830100	-0.47766200
Rh	-0.53108400	-0.33483700	1.44935200
Rh	0.54229800	-1.14710700	-0.76531200
N	1.90444900	1.99890300	0.01793200
O	3.21403700	-2.07751400	0.32104500
C	2.22415700	-1.75140700	-0.12474100
O	2.99830700	1.99657100	0.32984400

$^5ONRh_4^+CO$

Rh	0.37241400	1.34220600	-0.54549700
Rh	-1.91072200	-0.01596500	-0.48333100
Rh	-0.62624700	-0.10366400	1.47565900
Rh	0.45331100	-1.28654800	-0.59877400
N	2.00820600	1.82150900	-0.01894400
O	3.26076300	-1.82909600	0.30994900
C	2.20221800	-1.65601500	-0.06421500
O	2.95614200	1.83712100	0.60946600

$(ON)_bRh_4^+CO$



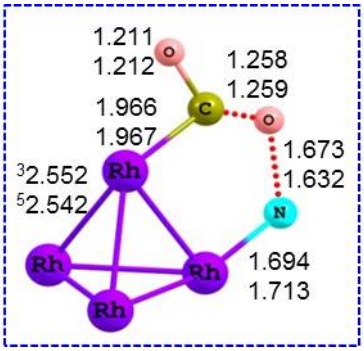
$^3(ON)_bRh_4^+CO$

Rh	0.09501300	0.45105300	1.53949000
Rh	1.52094800	-1.07500100	0.00859800
Rh	0.41271400	0.78358800	-1.40172100
Rh	-1.11738000	-0.98010100	-0.18995400
N	0.36145200	1.72225100	0.20257900
O	-3.81162800	0.35846200	-0.14968100
C	-2.81795700	-0.19015600	-0.17136500
O	0.48278900	2.89227700	0.34612500

$^5(ON)_bRh_4^+CO$

Rh	-0.50289800	-0.57388700	1.35572900
Rh	-0.97373700	1.56957700	-0.03284600
Rh	-0.46219800	-0.65883500	-1.33354600
Rh	1.51521000	0.56505100	-0.01795800
N	-1.54808900	-1.35399500	0.00709400
O	3.89773600	-1.33368400	0.08711400
C	3.04330500	-0.59100500	0.04290900
O	-2.44275700	-2.11153200	0.03548300

TS4-1



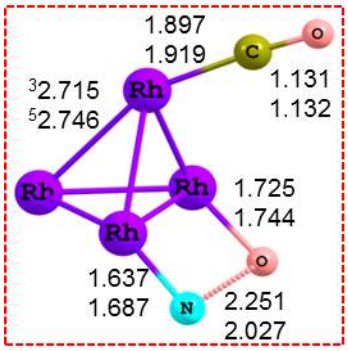
^{3}TS4-1 (-395.1 i)

Rh	-0.03518100	-0.03681700	0.02029100
Rh	0.07778300	0.01497800	2.63862400
Rh	2.18727600	-0.06592900	1.34980400
Rh	0.70710200	-2.14434200	1.41080200
N	-0.47534700	-0.93185000	-1.34854000
O	1.04901500	-3.91809100	0.02699600
O	0.04828500	-2.51514200	-1.48710100
C	0.52207700	-2.91076600	-0.39063100

^{5}TS4-1 (-383.0 i)

Rh	0.10030200	-0.00324800	-0.01295800
Rh	-0.14745100	-0.25361200	2.55351100
Rh	2.24589400	0.17551500	1.42835700
Rh	1.09345600	-2.08695000	1.30678500
N	-0.38462000	-0.92121300	-1.37523300
O	0.84525000	-3.97116000	0.08846100
O	-0.12032000	-2.53121500	-1.41202600
C	0.44849900	-2.91607700	-0.35665200

TS4-2



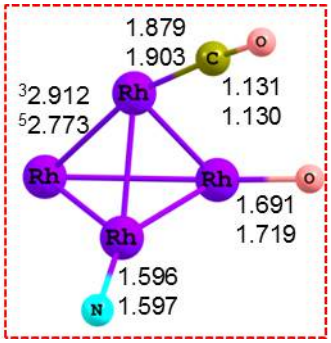
^{3}TS4-2 (-175.7 i)

Rh	-0.37303100	1.60571700	0.32248800
Rh	-1.62071400	-0.33629600	-0.86531800
Rh	-0.10708200	-1.35875000	0.82179600
Rh	1.07941800	-0.08152700	-0.98034200
N	-0.39540700	1.64772800	1.93945900
O	3.88883100	0.12815600	0.12417900
C	2.85841400	0.04167400	-0.33402900
O	0.05877200	-0.64011100	2.37456300

^{5}TS4-2 (-338.0 i)

Rh	0.48974600	1.62361400	0.51064900
Rh	-1.52981700	0.58990200	-0.81648300
Rh	-0.92477000	-1.53616500	0.50540900
Rh	1.02039600	-0.42488800	-0.90162600
N	0.04595700	1.26010700	2.04381000
O	3.77412200	-1.02415300	0.25938000
C	2.77833000	-0.79731700	-0.22845100
O	-0.58557700	-0.90056000	2.07265700

NRh_4^+OCO



$^{3}NRh_4^+OCO$

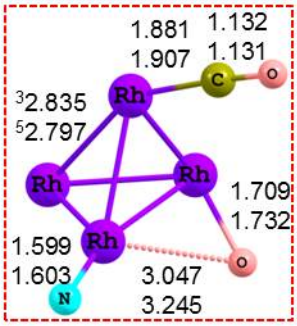
Rh	-0.28908000	1.35192800	0.64753700
Rh	-1.75678700	-0.18162000	-0.78490800
Rh	-0.05303100	-1.44082300	0.54579300
Rh	1.13188100	0.11986200	-1.03165400
N	-0.52813400	2.78447600	1.30996400
O	3.82185000	0.06189000	0.31452500
C	2.82818700	0.08945100	-0.22504300

O	-0.04140000	-1.71797000	2.21371600

$^5NRh_4^+OCO$

Rh	-0.45227200	1.18277800	0.78490600
Rh	-1.94259500	-0.53766700	-0.68171300
Rh	0.51373800	-1.24393700	0.87768800
Rh	0.68376400	0.17778600	-1.20908700
N	-0.93552000	2.47927600	1.58223700
O	3.60795200	0.92465200	-0.93284700
C	2.52520500	0.63996700	-1.08374600
O	2.05190200	-1.20564100	1.64485700

TS4-3



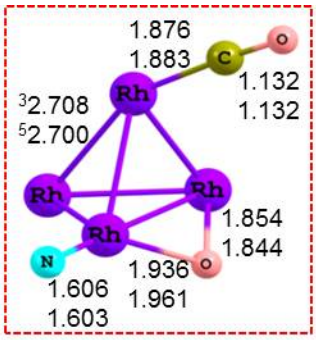
^{3}TS4-3

Rh	-0.28437600	1.37800000	0.60059500
Rh	-1.69733300	-0.21315400	-0.83045800
Rh	-0.07637400	-1.45945300	0.65546500
Rh	1.12147100	0.02415600	-1.01651200
N	-0.48687900	2.91845900	0.97671700
O	3.82327500	0.06162800	0.31362500
C	2.82793500	0.05383300	-0.22468000
O	-0.24976600	-1.13436900	2.32412600

^{5}TS4-3

Rh	0.13632700	1.40397800	0.57626300
Rh	-1.53604100	0.24079600	-1.03770000
Rh	-0.62020700	-1.41697500	0.70167700
Rh	1.20069600	-0.30934900	-0.85969000
N	0.28145600	2.86917200	1.21048500
O	3.88143700	-0.72036400	0.50440200
C	2.90176300	-0.58541400	-0.04410400
O	-1.69589200	-0.89237900	1.95390600

$NRh_4^+O_bCO$



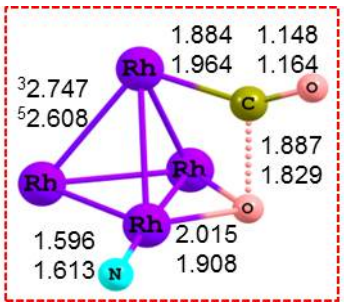
$^3NRh_4^+O_bCO$

Rh	-0.36766500	1.46971700	0.43975000
Rh	-1.62934100	-0.51233800	-0.77349100
Rh	0.03664100	-1.36340900	0.98679500
Rh	1.04784600	-0.17268100	-0.99237200
N	-0.64228700	3.01760600	0.10934800
O	3.79053400	0.30022800	0.14420500
C	2.77706300	0.11583500	-0.32539500
O	-0.17840800	0.22773700	1.91282600

$^5NRh_4^+O_bCO$

Rh	-0.61717500	1.41597300	0.43724500
Rh	-1.51839900	-0.71906600	-0.79691900
Rh	0.22166500	-1.35380200	0.97925500
Rh	1.07787700	0.00138300	-0.96936800
N	-1.11422500	2.91428700	0.16084600
O	3.79747700	0.65473000	0.15408500
C	2.79519100	0.40427600	-0.30939500
O	-0.21624900	0.17931200	1.90477200

TS4-4



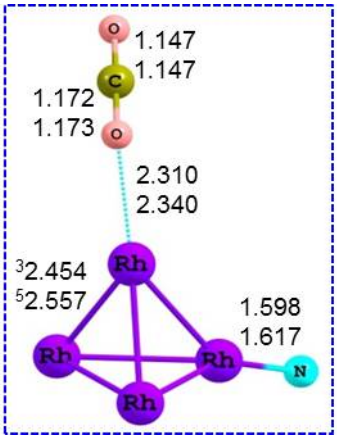
^{3}TS4-4 (-395.7 i)

Rh	0.09372100	1.53542400	-0.31969900
Rh	1.75009600	-0.33831600	0.41571500
Rh	-0.03773000	-1.31130200	-1.07143900
Rh	-0.85007000	-0.48192600	1.29003600
N	0.50948800	3.06409400	-0.13007600
O	-3.22888700	0.30700900	-0.19599000
C	-2.12420000	0.08403200	0.02315600
O	-1.00136500	0.30205800	-1.47725600

^{5}TS4-4 (-426.6 i)

Rh	-1.23749200	-0.89157500	-0.52786100
Rh	-0.73482100	1.61383200	0.17604900
Rh	1.34053500	0.58130600	-0.90871000
Rh	0.37102200	-0.34527600	1.49546500
N	-2.75970200	-1.37292200	-0.29925300
O	2.34482000	-1.97268300	0.21581000
C	1.48560600	-1.19352600	0.11864800
O	0.42246700	-1.32122900	-1.36450300

$NRh_4^+CO_2$



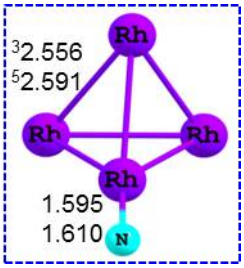
$^3NRh_4^+CO_2$

Rh	-0.77893200	1.45500100	-0.08906500
Rh	-1.58804000	-0.90552600	-0.68611700
Rh	-0.34671700	-0.52358500	1.50935700
Rh	0.85152800	-0.57337800	-0.63203500
N	-1.03206700	3.02478200	-0.24556700
O	3.14352700	-0.32497400	-0.49469400
O	5.12702800	0.63479100	0.22947700
C	4.14288200	0.16415100	-0.12594300

$^5NRh_4^+CO_2$

Rh	0.43895700	1.45795100	-0.00889200
Rh	1.23951700	-0.52829000	1.35143100
Rh	1.26076800	-0.54603000	-1.33004100
Rh	-0.90484800	-0.84819900	-0.00386000
N	0.20919700	3.05891900	-0.02628800
O	-3.23378500	-0.62557900	-0.05558500
O	-5.21768100	0.57311900	0.03636600
C	-4.23339400	-0.01453700	-0.00849600

NRh_4^+



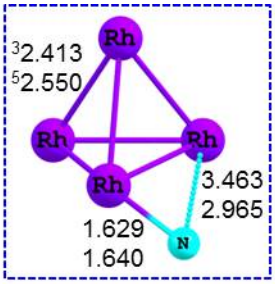
$^3NRh_4^+$

Rh	1.51099900	0.00112800	0.09203700
Rh	-0.84182200	-0.00130500	1.33482300
Rh	-0.57398100	-1.27816800	-0.73639400
Rh	-0.57648100	1.27821000	-0.73511900
N	3.09396600	0.00086700	0.28705800

$^5NRh_4^+$

Rh	-1.47294700	0.00061800	0.00663700
Rh	0.64815500	1.32500100	-0.69589100
Rh	0.64506400	-1.26396600	-0.80280000
Rh	0.65932600	-0.06216200	1.49069900
N	-3.08313000	0.00327700	0.00871300

TS4-5



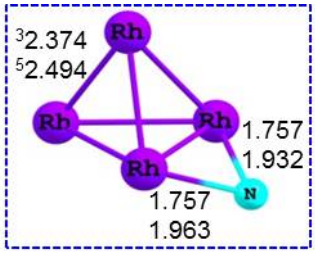
^{3}TS4-5(-106.0 i)

Rh	1.51973400	-0.17749200	0.54791400
Rh	-0.32446300	-1.17301300	-0.88687300
Rh	-0.28733400	1.34936600	-0.65671900
Rh	-1.36903900	-0.06311300	0.98322000
N	2.96423100	0.41304800	0.08008900

^{5}TS4-5(-99.3 i)

Rh	-0.26860400	1.58702700	-0.15150800
Rh	-0.87005400	-0.46597000	1.29118900
Rh	1.47407000	-0.52688400	0.08754500
Rh	-0.73236100	-0.70451400	-1.24394000
N	2.55181800	0.70933100	0.10744200

$N_bRh_4^+$



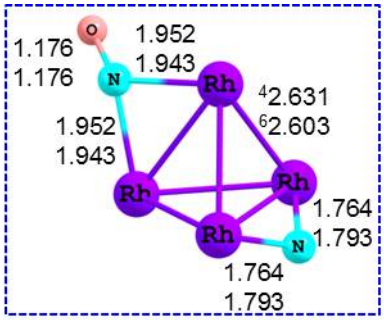
$^{3}N_bRh_4^+$

Rh	1.67471400	0.42436900	-0.00200900
Rh	-0.28622300	-0.93124500	-1.18510800
Rh	-1.18398300	1.16325400	-0.00142400
Rh	-0.28378800	-0.92578600	1.18883500
N	0.50966000	1.73190700	-0.00189000

$^{5}N_bRh_4^+$

Rh	-1.46535900	0.83531500	-0.05474500
Rh	-0.00537900	-0.88108800	1.30240000
Rh	1.47178800	0.82564900	-0.05138900
Rh	-0.00210300	-1.05905000	-1.18532700
N	0.00677200	1.79469000	-0.07032600

$N_bRh_4^+(NO)_b$



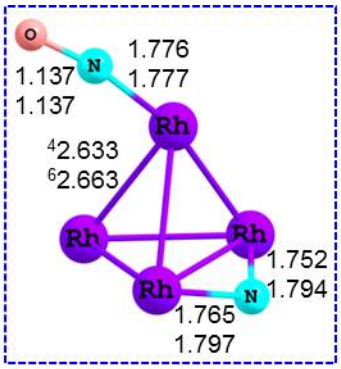
$^{4}N_bRh_4^+(NO)b$

Rh	0.68457400	-0.22329900	1.29803700
Rh	0.68477200	-0.22823400	-1.29762900
Rh	-0.58995300	1.67480300	-0.00226300
Rh	-1.37959100	-1.20191200	0.00188900
N	-1.89235800	0.48542700	-0.00196700
N	2.10822500	-0.54035800	0.00115900
O	3.18722500	-0.07207000	0.00051200

$^{6}N_bRh_4^+(NO)b$

Rh	0.64288000	-0.13524000	1.32119700
Rh	0.64297400	-0.13868300	-1.32017200
Rh	-0.63237100	1.70760000	-0.00172900
Rh	-1.24126400	-1.35250800	0.00103800
N	-1.82608300	0.34293700	-0.00110300
N	2.00619000	-0.55191900	0.00080200
O	3.14867200	-0.27371600	-0.00161400

$N_bRh_4^+NO$



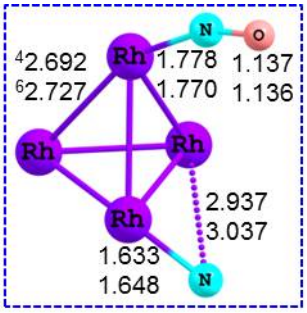
$^{4}N_bRh_4^+NO$

Rh	0.39107500	-0.22651400	1.37218800
Rh	-1.19992900	0.05175300	-0.70753700
Rh	1.03145400	-1.36061700	-0.87241700
Rh	0.96604800	1.57305300	-0.41005000
N	1.63259300	0.22101000	-1.32877900
N	-2.57410900	1.00938800	-0.11683600
O	-3.33867000	1.48928200	0.57496700

$^{6}N_bRh_4^+NO$

Rh	0.48808800	-0.23381200	1.33874800
Rh	-1.15193900	0.09370000	-0.73414100
Rh	0.99959200	-1.43303400	-0.81948500
Rh	0.99552200	1.63955000	-0.34029500
N	1.47161800	0.21963000	-1.33350500
N	-2.53599800	1.03392600	-0.13631800
O	-3.35842100	1.43739400	0.53653200

TS5-1



^{4}TS5-1 (-144.6 i)

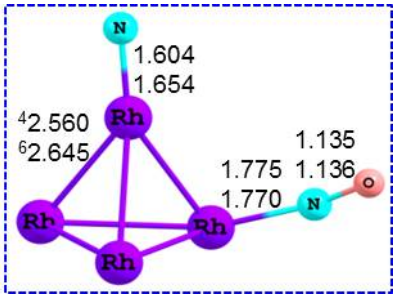
Rh	1.00436800	-1.33593300	0.94057400
Rh	-1.37159700	-0.16189600	0.46598700
Rh	0.37906900	-0.88464200	-1.41717200
Rh	0.91901700	1.11560600	0.38823800
N	1.61702400	1.73772200	-0.95058500
N	-2.50350700	1.08982700	-0.09271800
O	-2.90616600	2.03878200	-0.57136500

^{6}TS5-1 (-124.1 i)

Rh	1.01322900	-1.35943700	0.81320000
Rh	-1.40556700	-0.12573000	0.56475100
Rh	0.27098300	-0.82129500	-1.37063300

Rh	0.90803100	1.24487700	0.33383500
N	1.93379600	1.67242000	-0.88296100
N	-2.55670400	1.06365900	-0.06119200
O	-3.02555900	1.92497200	-0.63404000

NRh_4^+NO



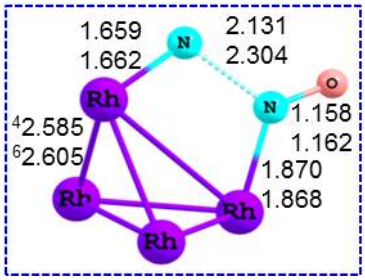
$^4NRh_4^+NO$

Rh	1.05489600	-1.20735200	0.88333600
Rh	-1.42577700	-0.16280600	0.55338600
Rh	0.27419500	-0.68796600	-1.42841500
Rh	0.77300600	1.25616900	0.24657400
N	1.55298400	2.65040000	0.39068300
N	-2.59786200	1.03357200	-0.03516300
O	-3.05803700	1.89508100	-0.61408800

$^6NRh_4^+NO$

Rh	1.04374100	-0.92071900	0.94522500
Rh	-1.47581800	-0.12146100	0.49652000
Rh	0.37725300	-0.49421600	-1.37539600
Rh	0.62928800	1.59787600	0.25089000
N	2.19953800	2.10040500	0.38020600
N	-2.78937800	0.90496500	-0.09743800
O	-3.41121900	1.71024800	-0.60369300

TS5-2



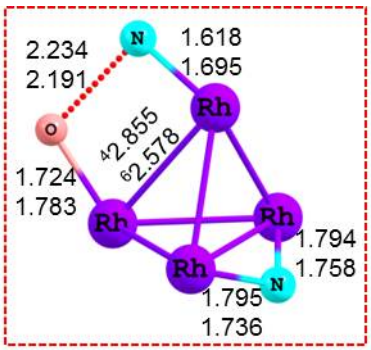
^{4}TS5-2 (-114.5 i)

Rh	0.00604200	-0.21726000	0.09383000
Rh	-0.08820900	0.49830500	2.57751200
Rh	2.19119500	-0.14778100	1.53982700
Rh	1.04593800	-2.40250800	1.00261300
N	0.17546600	-2.84890200	2.34284200
N	-0.55983300	-1.13035200	3.36582400
O	-1.20470000	-1.12453500	4.32817100

^{6}TS5-2 (-80.1 i)

Rh	-0.02593800	-0.22233700	0.15547200
Rh	-0.09587200	0.53197600	2.61886600
Rh	2.17215100	-0.22334900	1.60949600
Rh	1.07876700	-2.47038800	0.86964100
N	0.25554700	-2.90573200	2.24649200
N	-0.58504000	-1.09511400	3.39596300
O	-1.23371600	-0.98808900	4.35468900

TS5-3



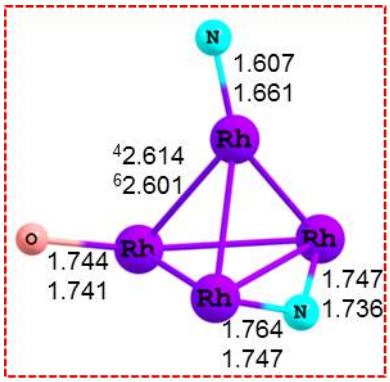
^{4}TS5-3 (-222.6 i)

Rh	-0.67937600	-1.51871200	0.46052200
Rh	-1.16625500	1.35513500	-0.40294400
Rh	0.62850600	-0.25122800	-1.41263600
Rh	0.54571700	0.55605100	1.32411100
N	2.21021700	0.05798200	-1.27213100
O	2.21091400	0.70493700	0.90130000
N	-1.85851800	-0.25807600	-0.03077300

^{6}TS5-3 (-253.7 i)

Rh	-1.22794400	-1.61766900	0.58574800
Rh	-0.85163200	1.31468500	-0.48431900
Rh	0.80147300	-0.59371100	-1.23859200
Rh	0.70739900	0.10088700	1.24279100
N	2.12166800	0.46619300	-1.31237800
O	2.13658500	1.06857200	0.79442100
N	-1.79634300	-0.09286500	-0.02022200

$(N)_b(N)$ Rh_4^+O



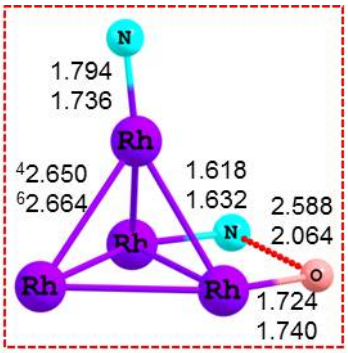
$^4(N)_b(N)Rh_4^+O$

Rh	0.06121100	-0.59616700	1.54953500
Rh	-1.33729800	-1.00830900	-1.15688800
Rh	1.15371500	-0.51362000	-0.81168500
Rh	-0.45124300	1.40780600	-0.06056900
N	2.49785600	-0.32103400	-1.67058700
O	0.52589400	2.63856800	0.69599700
N	-1.22644800	-1.29027700	0.56413600

$^{6}(N)_{b}(N)Rh_{4}^{+}O$

Rh	0.26483600	-1.44360800	1.31990700
Rh	-1.73724100	-0.07858900	-0.75445300
Rh	1.12942200	-0.61976900	-0.99431400
Rh	0.11152400	1.22894200	0.52561700
N	2.73809700	-0.20619800	-0.98408200
O	-0.05284000	2.66450400	-0.44562900
N	-1.23011000	-1.22831600	0.44289200

TS5-4



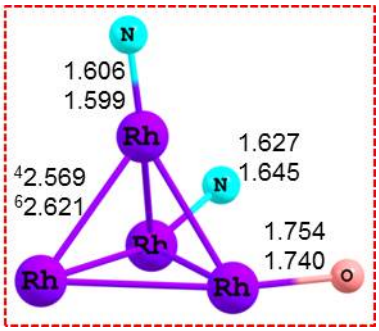
^{4}TS5-4 (-83.7 i)

Rh	1.21789600	-1.15353400	0.56058700
Rh	0.86245300	1.24922600	-0.32989700
Rh	-0.94728800	0.04169500	1.36043500
Rh	-0.79360100	-0.46931500	-1.26724300
N	-2.44364500	0.69264900	1.24348800
O	-2.32926600	0.29000900	-1.59662100
N	1.89304500	2.43369800	-0.65779900

^{6}TS5-4 (-188.4 i)

Rh	1.52556000	-1.36548000	0.18184200
Rh	0.82914400	1.17142500	-0.23456200
Rh	-0.99205400	0.20048600	1.34753000
Rh	-0.78597400	-0.57944300	-1.15193200
N	-2.42161200	0.90986800	0.88761200
O	-2.33268800	0.22096900	-1.31685500
N	1.75937500	2.45420600	-0.45442500

$(N)_{2}Rh_{4}^{+}O$



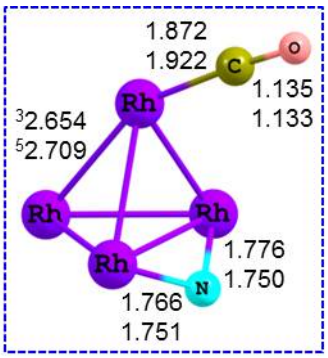
$^{4}(N)_{2}Rh_{4}^{+}O$

Rh	-0.86880900	0.46409800	1.42749500
Rh	0.37725300	1.21877600	-0.68858900
Rh	-1.44437600	-0.77420200	-0.71465000
Rh	1.53111200	-0.71365700	0.50065500
N	-0.93304100	-2.26772900	-1.10892700
O	2.58818100	-1.40542000	-0.71676900
N	0.57753800	2.62025200	-1.44633800

$^{6}(N)_{2}Rh_{4}^{+}O$

Rh	-1.77470200	-0.62522200	-0.79505700
Rh	-0.55218500	1.08575000	0.76926000
Rh	1.22690200	0.44272100	-1.13859600
Rh	0.54242000	-1.22487700	0.72148200
N	2.52011400	1.32713600	-0.63776300
O	2.02525000	-1.31381100	1.62663400
N	-1.25034100	2.24196600	1.62604700

$N_{b}Rh_{4}^{+}CO$



$^{3}N_{b}Rh_{4}^{+}CO$

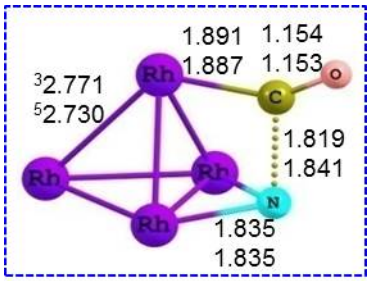
Rh	1.52533100	-0.56003500	0.11564600
Rh	-0.71542200	-1.16678200	-0.95553300
Rh	-0.51247500	1.42716500	-0.62261200
Rh	-0.63538300	-0.10169100	1.47391400
N	1.21376800	1.07933600	-0.49161600
C	-0.17297800	-1.43122700	-2.72760300
O	0.20518200	-1.53772900	-3.79190700

$^{5}N_{b}Rh_{4}^{+}CO$

Rh	1.57641600	-0.50324600	0.27266900
Rh	-0.63205100	-1.14126300	-0.99441600

Rh	-0.51149500	1.44759100	-0.58084100
Rh	-0.64395400	-0.06576000	1.49222200
N	1.18685300	1.04821500	-0.43749600
C	-0.19303900	-1.47377700	-2.83633100
O	0.12529200	-1.60272100	-3.91551900

TS6-1



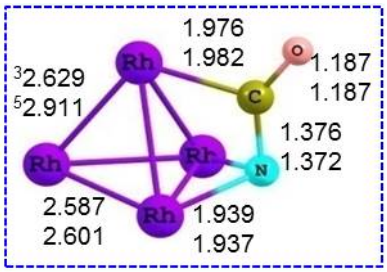
^{3}TS6-1 (-488.1 i)

Rh	-0.05522500	-0.85184900	1.32597300
Rh	-0.05742300	-0.85443800	-1.32367800
Rh	1.90310600	0.44083700	-0.00214700
Rh	-0.70017900	1.38972800	0.00004400
N	-1.25306400	-1.27859700	0.00231700
C	-2.21877800	0.26263000	-0.00048700
O	-3.37230500	0.22274000	-0.00273800

^{5}TS6-1 (-501.8 i)

Rh	0.06627700	1.28559200	0.25157900
Rh	-1.52417600	-0.39339700	-1.06320000
Rh	-1.24148100	-0.63872900	1.59784500
Rh	0.82191100	-1.28790400	-0.06752000
N	-0.20942900	0.81017300	-1.49917800
C	1.18781900	-0.37489600	-1.67794500
O	1.87973100	-0.31076300	-2.59764800

$Rh_4^+N_bCO$



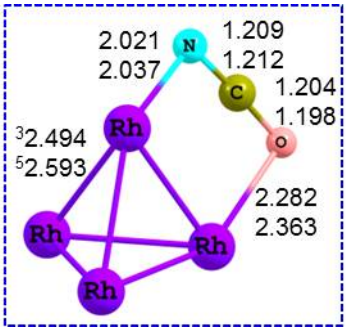
$^3Rh_4^+N_bCO$

Rh	-0.37402200	-1.49323700	-0.78758900
Rh	0.43213100	1.57022400	-0.59149400
Rh	1.59303900	-0.37230500	0.37120500
Rh	-0.76692800	0.01262900	1.30453900
N	-0.86958800	0.31912900	-1.37783100
C	-1.76630900	0.54802000	-0.36096400
O	-2.88811700	0.89987100	-0.19239100

$^5Rh_4^+N_bCO$

Rh	-0.00017100	-0.89084500	-1.32343000
Rh	-0.00186900	-0.88792700	1.32556700
Rh	-1.72728400	0.51413900	-0.00185300
Rh	0.68489900	1.39890700	-0.00026400
N	1.36565700	-1.24251800	0.00254500
C	2.03626300	-0.04073800	-0.00001200
O	3.15274300	0.36246700	-0.00232900

Rh_4^+NCO



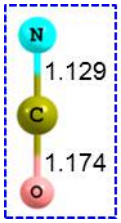
$^3Rh_4^+NCO$

Rh	0.72608900	-1.06325700	-0.75903900
Rh	-0.68978700	-0.69686500	1.26082800
Rh	-1.75883200	0.35021900	-0.67454100
Rh	0.46149400	1.29636300	0.10407000
N	2.68772600	-0.94423800	-0.28669000
C	2.72131700	0.19231600	0.12503400
O	2.70057300	1.32063600	0.54341700

$^5Rh_4NCO$

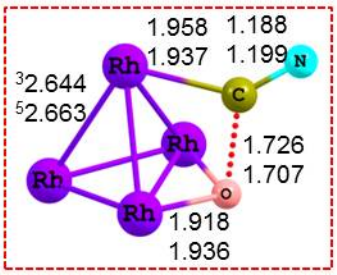
Rh	0.60396700	-1.11027000	-0.73323000
Rh	-0.82331300	-0.56444000	1.36145500
Rh	-1.66785100	0.36639500	-0.78013400
Rh	0.59920200	1.32254400	0.08170600
N	2.57226300	-1.22357900	-0.22064000
C	2.77793000	-0.08246000	0.13118100
O	2.91078900	1.05243800	0.48957200

NCO



N	-3.74389100	0.30160200	0.00000000
C	-2.52601000	0.36018800	0.00000000
O	-1.35291600	0.41561600	0.00000000

TS6-2



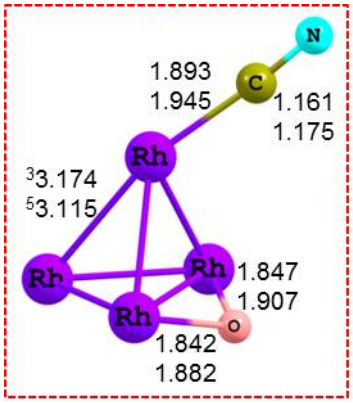
^{3}TS6-2 (-551.6 i)

Rh	-0.40152800	-0.25878200	-0.02617300
Rh	-0.84841600	-0.29942500	2.47268200
Rh	1.84765300	0.71248100	1.18814600
Rh	1.15302600	-1.62535300	1.61860900
N	-0.69733100	2.63891600	0.21150600
C	-0.35319100	1.58330000	0.63523300
O	0.27078100	1.23501000	2.20605800

^{5}TS6-2 (-640.9 i)

Rh	-0.10874000	-0.18866700	-0.18474000
Rh	-0.87415600	-0.09083200	2.38489400
Rh	1.97669600	0.57408900	1.20156100
Rh	0.97928100	-1.68846600	1.72775300
N	-1.00375300	2.55838400	0.42423200
C	-0.44238100	1.52437100	0.65556700
O	0.44404700	1.29726700	2.09679400

$O_bRh_4^+CN$



$^{3}O_bRh_4^+CN$

Rh	1.15803800	0.01152200	1.06592900
Rh	-0.07887700	-1.46510300	-0.54323700
Rh	-0.10027100	1.46597100	-0.54841300
Rh	-1.89613400	-0.01145000	0.45435800
N	3.59268500	-0.00806400	-0.78072300
C	2.66584900	0.00249000	-0.08298400
O	0.01650800	-0.00009600	-1.66570800

$^{5}O_bRh_4^+CN$

Rh	-1.19188100	0.01223300	1.06998700
Rh	0.09382400	1.48640300	-0.54679000
Rh	0.09319400	-1.46948800	-0.54622700
Rh	1.92204500	-0.01744000	0.45715200
N	-3.58977600	-0.06193800	-0.81913800
C	-2.67453000	-0.03091700	-0.10615700
O	-0.01219400	0.01152400	-1.64557400

CN

N	0.00000000	0.00000000	0.02459500
C	0.00000000	0.00000000	1.18692500

Table S8: IRC analysis for TS4-2 (5TS4-2 and 3TS4-2) and the geometries of the approximate crossing point.