

Supporting Information

Nitroxyl as a ligand in rutheniumtetraammine systems. A density functional theory study.

Augusto C. H. Da Silva, Juarez L. F. Da Silva, Douglas W. Franco.*

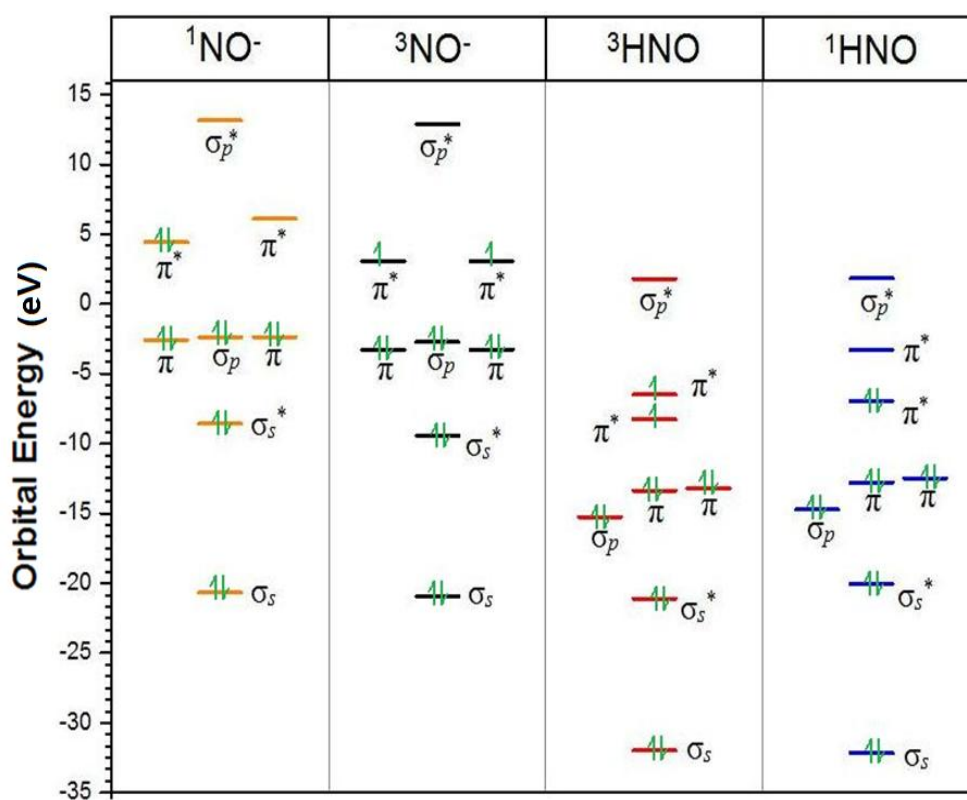


Figure S1: Nitroxyl species: B3LYP/DGDZVP valence molecular orbitals energies, occupancy and symmetry.

Table S1: Free Nitroxyl Species DFT calculated properties: Electronic Energies (E); N-O bond length (B.L._{N-O}); N-O bond stretching (ν_{N-O}); Mulliken Charges at nitrogen, oxygen and hydrogen (C_N , C_O , C_H respectively).

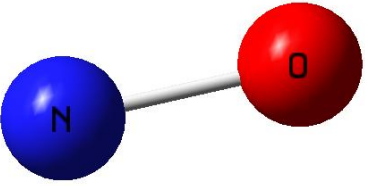
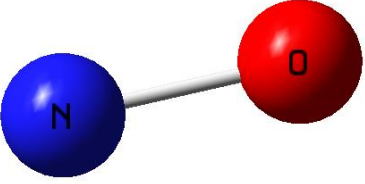
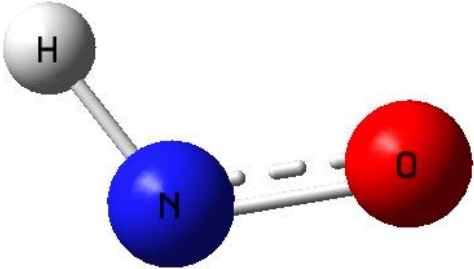
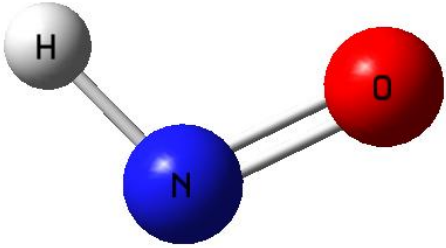
Spin= singlet	Charge= -1	ne⁻= 16		Gas phase	IEFPCM (water)
			E (u.a.)	-129.85845053	-129.98237140
			B.L._{N-O} (Å)	1.281	1.275
			ν_{N-O}	1435	1453
			C_N	-0.528	-0.540
			C_O	-0.472	-0.460
Spin= triplet	Charge= -1	ne⁻= 16		Gas phase	IEFPCM (water)
			E (u.a.)	-129.91108410	-130.03274590
			B.L._{N-O} (Å)	1.287	1.283
			ν_{N-O}	1420	1431
			C_N	-0.484	-0.486
			C_O	-0.516	-0.514
Spin= triplet	Charge= 0	ne⁻= 16		Gas phase	IEFPCM (water)
			E (u.a.)	-130.47795529	-130.48269174
			B.L._{N-O} (Å)	1.238	1.239
			B.L._{H-N} (Å)	1.033	1.034
			Angle (°)	118.45	119.21
			ν_{N-O}	1583	1586
			C_N	-0.228	-0.238
			C_O	-0.136	-0.166
			C_H	0.365	0.404
Spin= singlet	Charge= 0	ne⁻= 16		Gas phase	IEFPCM (water)
			E (u.a.)	-130.49366383	-130.49816660
			B.L._{N-O} (Å)	1.214	1.217
			B.L._{H-N} (Å)	1.065	1.057
			Angle (°)	108.14	108.35
			ν_{N-O}	1668	1661
			C_N	-0.133	-0.147
			C_O	-0.163	-0.192
			C_H	0.297	0.339

Table S2: Energy difference between the singlet and triplet species of coordinated nitroxyl and HOMO-LUMO energy gap.

Species	$s-t\Delta E_{el}$	$s-t\Delta G$	Singlet species
	(kcal.mol ⁻¹)		HOMO - LUMO gap (eV)
<i>trans</i> -[Ru(NH ₃) ₅ NO] ¹⁺	-9,3	-8,5	3.31
<i>trans</i> -[Ru(NH ₃) ₄ (py)NO] ¹⁺	-8,5	-7,4	3.03
<i>trans</i> -[Ru(NH ₃) ₄ (P(OEt) ₃)NO] ¹⁺	-1,0	-1,3	3.0
<i>trans</i> -[Ru(NH ₃) ₄ (H ₂ O)NO] ¹⁺	-10,3	-9,5	3.48
<i>trans</i> -[Ru(NH ₃) ₄ (Cl)NO]	-11,1	-10,5	3.41
<i>trans</i> -[Ru(NH ₃) ₅ HNO] ²⁺	-32,1	-30,4	3.69
<i>trans</i> -[Ru(NH ₃) ₄ (py)HNO] ²⁺	-29,0	-27,9	6.37
<i>trans</i> -[Ru(NH ₃) ₄ (P(OEt) ₃)HNO] ²⁺	-35,8	-32,5	3.37
<i>trans</i> -[Ru(NH ₃) ₄ (H ₂ O)HNO] ²⁺	-34,3	-32,8	3.82
<i>trans</i> -[Ru(NH ₃) ₄ (Cl)HNO] ¹⁺	-37,9	-35,4	3.56

Table S3: B3LYP/DGDZVP selected Mulliken charges, H-N_(HNO) distances and $\nu_{H-N(HNO)}$ stretching. for the free nitroxyl molecule, nitroxyl complexes series and pentacoordinated systems ¹[Ru(NH₃)₄(L)]ⁿ⁺.

Species	Mulliken Charges				D	ν
	Ru	Ru _(5cdt)	H _{HNO}	N _{HNO}	H-N(HNO)	H-N(HNO)
Free HNO	#	#	0.339	-0.147	1.07	3007.6
¹ [Ru(NH ₃) ₅ HNO] ²⁺	1.063	1.013	0.391	-0.241	1.04	3204.0
<i>trans</i> - ¹ [Ru(NH ₃) ₄ (py)HNO] ²⁺	1.039	1.24	0.390	-0.231	1.04	3199.4
<i>trans</i> - ¹ [Ru(NH ₃) ₄ (P(OEt) ₃)HNO] ²⁺	0.640	0.538	0.394	-0.237	1.04	3189.6
<i>trans</i> - ¹ [Ru(NH ₃) ₄ (Cl)HNO] ¹⁺	0.841	0.834	0.382	-0.240	1.04	3206.8
<i>trans</i> - ¹ [Ru(NH ₃) ₄ (Br)HNO] ¹⁺	0.865	0.871	0.384	-0.237	1.04	3196.3
<i>trans</i> - ¹ [Ru(NH ₃) ₄ (H ₂ O)HNO] ²⁺	1.051	1.033	0.398	-0.229	1.04	3216.8

Table S4: NBO 3.0 and NBO 6.0 orbital energies data for Ru-N(H)O bond.

Species	NBO 3.0	NBO 6.0 (a.u.)
$^1[\text{Ru}(\text{NH}_3)_5\text{HNO}]^{2+}$	σ -0.65611	σ -0.64826
$^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{py})\text{HNO}]^{2+}$	σ -0.67531 π -0.33628	σ -0.66753 π -0.32362
$^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{P}(\text{OEt})_3)\text{HNO}]^{2+}$	σ -0.66005	σ -0.64364
$^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{Cl})\text{HNO}]^{1+}$	σ -0.65586	σ -0.64299
$^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{Br})\text{HNO}]^{1+}$	σ -0.65800	σ -0.64418
$^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{H}_2\text{O})\text{HNO}]^{2+}$	σ -0.67219	σ -0.65661

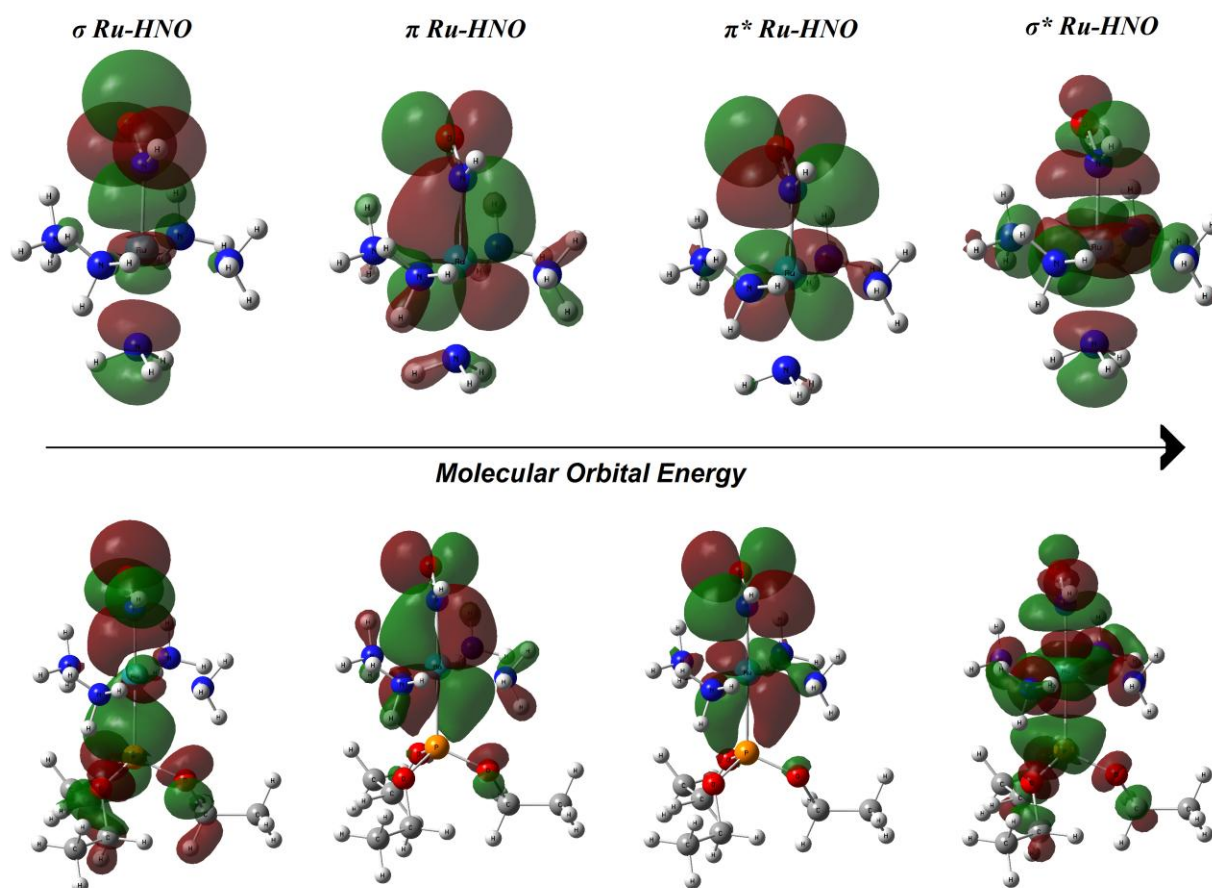


Figure S2: Ru-HNO σ and π bonding and anti bonding molecular orbitals isosurfaces for the $^1[\text{Ru}(\text{NH}_3)_5\text{HNO}]^{2+}$ (above) and $^{\text{trans-}}^1[\text{Ru}(\text{NH}_3)_4(\text{P}(\text{OEt})_3)\text{HNO}]^{2+}$ (below).

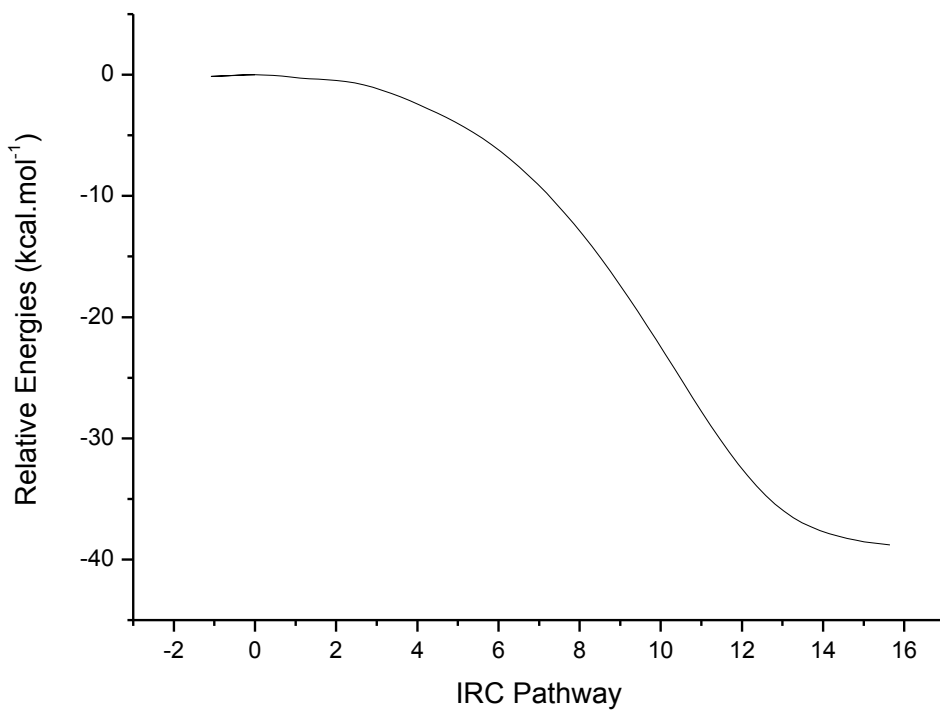


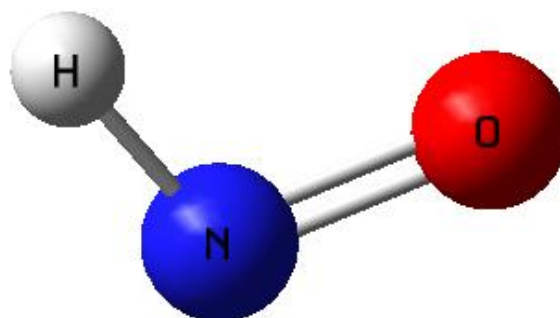
Figure S3: IRC pathway to the HNO cleavage in $^1[\text{Ru}(\text{NH}_3)_5\text{HNO}]^{2+}$ system.

Geometry Index:

Free HNO structures: B3LYP/DGDZVP

^1HNO

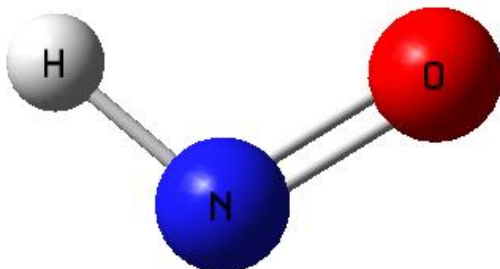
0 1			
N	0.06271200	0.58785100	0.00000000
O	0.06271200	-0.62944600	0.00000000
H	-0.94068000	0.92060900	0.00000000



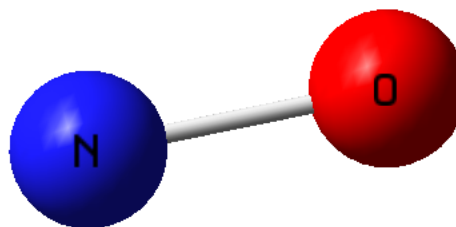
2 Lower vibrational modes in $1572.1181 \text{ cm}^{-1}$ and $1667.8745 \text{ cm}^{-1}$.

^3HNO

0 3			
N	0.05642500	0.58799600	0.00000000
O	0.05642500	-0.65110200	0.00000000
H	-0.84637600	1.09284300	0.00000000



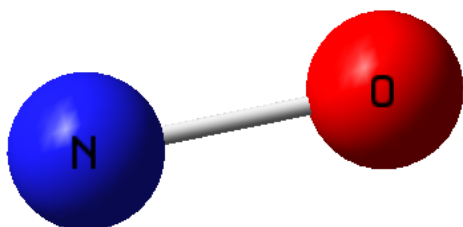
2 Lower vibrational modes in 1068.4783 cm^{-1} and 1583.4498 cm^{-1} .



Lower vibrational mode in 1420.4476 cm^{-1} .

^1NO

-1 1			
N	0.00000000	0.00000000	-0.68314900
O	0.00000000	0.00000000	0.59775500



Lower vibrational mode in 1435.2792 cm^{-1} .

^3NO

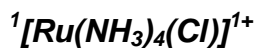
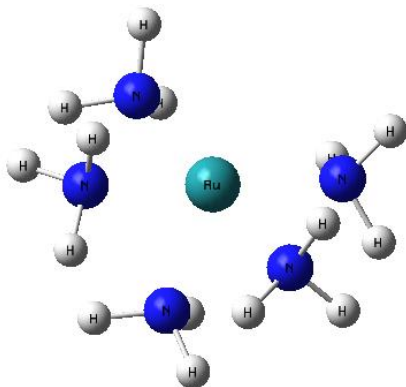
-1 3			
N	0.00000000	0.00000000	-0.68637000
O	0.00000000	0.00000000	0.60057300

HNO BDE structures and Enthalpies: B3LYP/DGDZVP
SCRF(IEFPCM,SOLVENT=WATER)



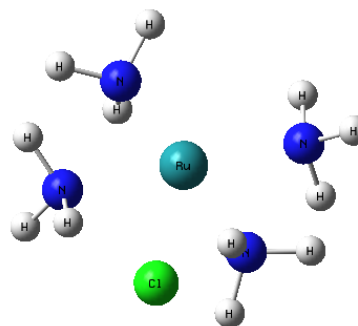
2 1			
Ru	0.00046900	-0.00006600	-0.21535300
N	-1.39466300	1.69253100	-0.25938200
N	-1.69066700	-1.39577300	-0.27660500
N	1.41207700	-1.67879000	-0.26358300
N	1.69007500	1.40240400	-0.24652800
H	-1.14612000	2.46389600	0.36430500
H	-1.43955500	2.10403000	-1.19478200
H	-2.36057400	1.45548900	-0.02149200
H	-1.96628700	-1.59748300	-1.24082000
H	-1.50975400	-2.30719300	0.15055800
H	-2.53792000	-1.05263100	0.18177700
H	1.00533100	-2.58612500	-0.02578700
H	1.80742400	-1.79681900	-1.19954600
H	2.21556100	-1.57323600	0.35998200
H	1.96357600	1.61556200	-1.20879200
H	1.50229300	2.30866500	0.18865500
H	2.54039200	1.05800900	0.20555200
N	-0.01988100	-0.02187200	1.90406800
H	0.09946200	-0.95959700	2.29516600
H	0.72180600	0.54806300	2.31783300
H	-0.89485900	0.33274700	2.29713100

2 Lower vibrational modes in 18.3926 cm^{-1} and 55.1075 cm^{-1} .
 Enthalpy = - 4725.272989 Hartree



1 1			
Ru	0.00244900	0.00662100	-0.42179000
N	1.38217500	1.70534500	-0.36547600
N	-1.69939200	1.38531600	-0.38751900
N	-1.37622400	-1.69482200	-0.42249300
N	1.70509600	-1.37035100	-0.40482000
H	1.35908000	2.13914100	0.56036100
H	2.35926900	1.45567700	-0.52739600
H	1.17680200	2.45185000	-1.03287000
H	-1.44371400	2.36163900	-0.54148700
H	-2.43236600	1.18591400	-1.07239300
H	-2.14684400	1.35985400	0.53152200
H	-2.34991800	-1.43219700	-0.58494900
H	-1.16849300	-2.42022900	-1.11253100
H	-1.36957600	-2.15478700	0.48946200
H	2.44403500	-1.15435900	-1.07698200
H	2.15012100	-1.36121300	0.51483400
H	1.45413000	-2.34463500	-0.58596800
Cl	-0.01305000	-0.03272900	2.00348900

2 Lower vibrational modes in 50.1486 cm^{-1} and 63.4725 cm^{-1} .
 Enthalpy = -5129.082081 Hartree



0 1			
N	0.06271200	0.58788200	0.00000000
O	0.06271200	-0.62944100	0.00000000
H	-0.94068600	0.92035400	0.00000000

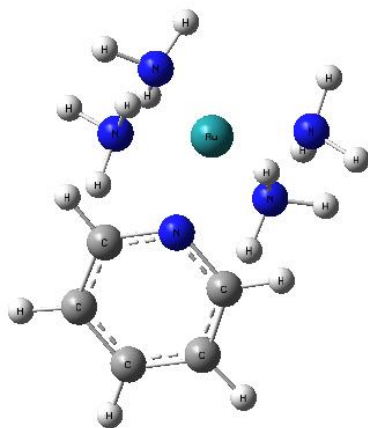
2 Lower vibrational modes in 1570.6298 cm^{-1} and 1660.6932 cm^{-1} .
 Enthalpy = -130.480169 Hartree

$^1[Ru(NH_3)_4(py)]^{2+}$

2 1			
Ru	1.13587300	0.00007600	0.00025700
N	1.19393500	1.43175300	-1.66081400
N	1.22041900	-1.60326900	-1.49734900
N	1.19231200	-1.43170500	1.66139300
N	1.21752400	1.60362200	1.49800000
H	0.35629500	1.41822800	-2.24759500
H	1.32341300	2.40910400	-1.38902700
H	1.97219000	1.23139200	-2.29372700
H	2.09573500	-1.55291400	-2.02494900
H	1.18963400	-2.55878500	-1.13338200
H	0.47815200	-1.55397300	-2.19909700
H	1.32353300	-2.40880900	1.38955200
H	1.96899300	-1.23059400	2.29599200
H	0.35343300	-1.41936200	2.24642000
H	2.09227300	1.55393600	2.02659900
H	1.18647300	2.55906900	1.13388700
H	0.47448200	1.55379500	2.19888200
N	-0.92259400	-0.00013900	-0.00064400
C	-1.62641800	1.15890300	-0.01315700
C	-3.01772000	1.19771800	-0.01290000
C	-3.73576400	-0.00020300	-0.00036800
C	-3.01765300	-1.19808700	0.01188500
C	-1.62634200	-1.15922600	0.01182900
H	-1.05169900	2.07683500	-0.02237600
H	-3.51798400	2.16069100	-0.02201200
H	-4.82167600	-0.00022400	-0.00017200
H	-3.51788800	-2.16107300	0.02107100
H	-1.05157200	-2.07713700	0.02080400

2 Lower vibrational modes in 54.1621 cm^{-1} and 74.4804 cm^{-1} .

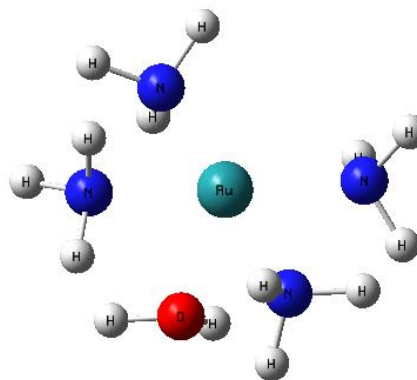
Enthalpy = -4916.959784 Hartree

 $^1[Ru(NH_3)_4(H_2O)]^{2+}$

2 1			
Ru	-0.00275800	0.00813600	-0.22781600
N	1.02889500	-1.91280400	-0.23701900
N	1.93418600	1.02533600	-0.29009200
N	-1.04810600	1.93454600	-0.17834600
N	-1.93567300	-1.02003100	-0.28984900
H	1.28134800	-2.18584800	0.71591400
H	0.47500500	-2.68586300	-0.61217800
H	1.90006700	-1.91981200	-0.77209700
H	2.21525300	1.20643800	-1.25685700
H	1.96064100	1.93517200	0.17581800
H	2.70061700	0.48922600	0.12318800
H	-0.43563800	2.74439700	-0.29871300
H	-1.74632200	2.01296900	-0.92163600
H	-1.55522500	2.10435100	0.69342700
H	-2.17503300	-1.27214200	-1.25188000
H	-1.97585000	-1.89473600	0.23861000
H	-2.72230000	-0.46198400	0.04983700
H	-0.78776400	-0.23268000	2.35647400
O	0.07886100	-0.12726600	1.92303100
H	0.50056200	0.63135400	2.36687800

2 Lower vibrational modes in 88.7813 cm^{-1} and 109.1886 cm^{-1} .

Enthalpy = -4745.134659 Hartree

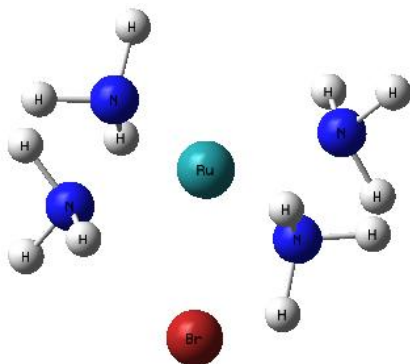


$^1[Ru(NH_3)_4(Br)]^{1+}$

1 1			
Ru	0.74965500	0.00098200	0.00072200
N	0.75486800	-1.66350600	1.42600200
N	0.74777200	1.42741100	1.66404800
N	0.75227100	1.66530700	-1.42474200
N	0.75830100	-1.42513800	-1.66264500
H	0.81498700	-2.58409000	0.98588400
H	1.52365000	-1.63083800	2.09927800
H	-0.10660200	-1.67959400	1.97652400
H	1.52051200	2.09663000	1.63996200
H	-0.11072800	1.98263100	1.66975400
H	0.79504700	0.98747700	2.58537800
H	1.51600500	1.62960800	-2.10368000
H	-0.11311700	1.68464200	-1.96889700
H	0.81954700	2.58573900	-0.98522900
H	1.53998800	-2.08387700	-1.64047200
H	-0.09256400	-1.99207600	-1.66559600
H	0.79608400	-0.98488600	-2.58412300
Br	-1.79943200	-0.00237400	-0.00169100

2 Lower vibrational modes in 64.2993 cm^{-1} and 85.9101 cm^{-1} .

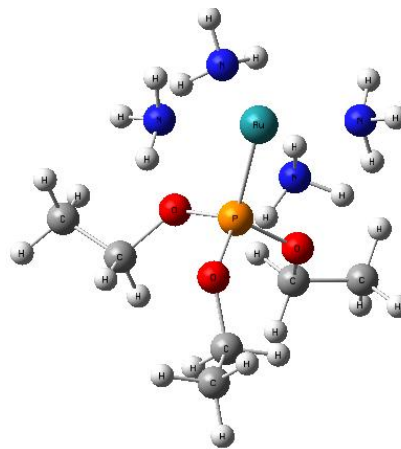
Enthalpy = -7242.612377 Hartree

 $^1[Ru(NH_3)_4(P(OEt)_3)]^{2+}$

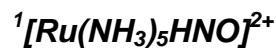
2 1			
Ru	-1.74581900	0.00368900	0.03424300
N	-1.85580300	0.01754600	-2.14835800
N	-1.89504900	2.18509700	0.08111900
N	-1.81056700	-0.06280700	2.21793200
N	-1.80386300	-2.18338000	-0.01813900
H	-2.74858100	-0.36435800	-2.47146900
H	-1.77992500	0.94219200	-2.57788500
H	-1.12623800	-0.54537000	-2.59195200
H	-0.98217200	2.64326800	0.13578100
H	-2.43621100	2.53141200	0.87674600
H	-2.35579000	2.57332800	-0.74507600
H	-1.67216900	0.84029500	2.67664900
H	-2.71610700	-0.40604500	2.54852200
H	-1.10522500	-0.68153800	2.62370100
H	-1.35346300	-2.64907800	0.77238700
H	-2.77687600	-2.50071600	-0.00749100
H	-1.38687800	-2.60166600	-0.85248100
P	0.44929000	0.02770500	0.00621400
O	1.09864700	-0.78710700	1.25246000
O	1.05726600	-0.64815300	-1.33970800
O	1.09345500	1.51831400	0.07240400
C	2.35515700	-0.46329600	1.93726500
C	2.39278600	-1.24110000	3.23939800
H	3.18910700	-0.74409100	1.28800500
H	2.38429300	0.61438300	2.11425900
H	3.32974600	-1.02093300	3.76138900
H	1.56069700	-0.95573900	3.88959600
H	2.34625000	-2.31824400	3.05471700
C	2.22038700	-1.53487700	-1.43681800
C	2.09732500	-2.32900200	-2.72379900
H	2.23373200	-2.19115300	-0.56366800
H	3.12324300	-0.91756700	-1.43685300
H	2.06762500	-1.66532800	-3.59284900
H	1.19320200	-2.94487800	-2.71629100
H	2.96554800	-2.98857500	-2.82310900
C	2.27500400	1.98885000	-0.65931100
C	2.24677700	3.50578300	-0.67365900
H	2.24254300	1.57797200	-1.67090200
H	3.16748500	1.61626200	-0.14886800
H	3.13314400	3.87444700	-1.20019300
H	1.35873900	3.87735800	-1.19340900
H	2.25837300	3.90868800	0.34324600

2 Lower vibrational modes in 15.0904 cm^{-1} and 26.5363 cm^{-1} .

Enthalpy = -5473.323943 Hartree



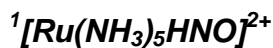
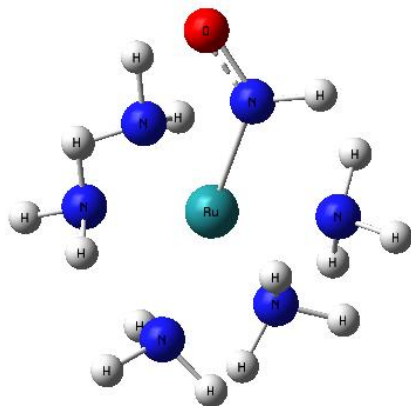
**HNO Simplest cleavage structures and Free Energies: B3LYP/DGDZVP
SCRF(IEFPCM,SOLVENT=WATER)**



RC

2 1			
Ru	-0.13483500	0.00329200	-0.00685300
N	0.64601400	1.00930300	1.75886400
H	0.43275000	0.53922200	2.64152200
H	1.66798600	1.05626000	1.70795700
N	-0.93909300	1.89126400	-0.78131100
H	-0.30243700	2.68194900	-0.65635300
H	-1.15624200	1.87859100	-1.78055100
N	-0.96012500	-1.06319000	-1.73575700
H	-0.26109200	-1.60245600	-2.25169800
H	-1.67990000	-1.73905700	-1.46957500
N	0.64806700	-1.85735400	0.80609700
H	1.66935000	-1.86116000	0.72689500
H	0.44532700	-2.00921200	1.79649300
N	-2.09842600	-0.33445600	1.03069600
H	-2.21479500	0.25178300	1.86044300
H	-2.92158100	-0.14922600	0.45271800
H	0.32555000	1.97309200	1.87964300
H	-1.80865600	2.16857300	-0.31947900
H	-2.21230300	-1.29426700	1.36496500
H	-1.40368300	-0.45906400	-2.43126300
H	0.32599600	-2.70142000	0.32625000
N	1.55073800	0.29047300	-0.87062200
O	2.68683700	0.11671300	-0.39350100
H	1.60155400	0.63555400	-1.85419700

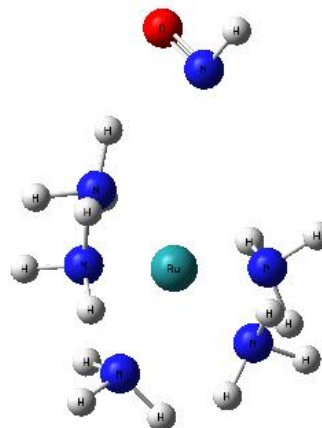
2 Lower vibrational modes in 15.3242 cm^{-1} and 82.8734 cm^{-1} .
Free Energy = - 4855.874174 Hartree

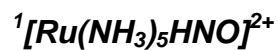


TS

2 1			
Ru	-0.38089000	-0.00006800	0.03661100
N	0.89432800	-0.50578400	-1.67241300
H	0.83167000	0.15503200	-2.45018800
H	1.88170400	-0.51283500	-1.39545900
N	-0.52997500	-2.11865900	0.57973900
H	-0.02372800	-2.31220200	1.44725300
H	-1.48243400	-2.45418500	0.74153400
N	-1.59709800	0.52551000	1.79267700
H	-1.06607700	1.08481000	2.46442100
H	-2.43106600	1.07705800	1.57865400
N	-0.16308200	2.13667800	-0.43151700
H	0.73870300	2.48695600	-0.10009900
H	-0.19596800	2.37236600	-1.42610100
N	-2.12020100	-0.13485200	-1.16677000
H	-1.94760100	-0.59395100	-2.06435600
H	-2.87680900	-0.66372200	-0.72609100
H	0.71708300	-1.42348800	-2.08822900
H	-0.13406300	-2.75929200	-0.11148000
H	-2.51930000	0.77919100	-1.39416100
H	-1.93552300	-0.28180400	2.32058300
H	-0.86547900	2.73354100	0.01135700
N	2.91790900	0.21988500	0.91985500
O	3.58597900	-0.12579600	-0.03561200
H	3.56703200	0.46243900	1.71536300

2 Lower vibrational modes in 30.1022 cm^{-1} and 56.8537 cm^{-1} .
1 Imaginary frequency in -109.8251 cm^{-1} .
Free Energy = -4855.817443 Hartree





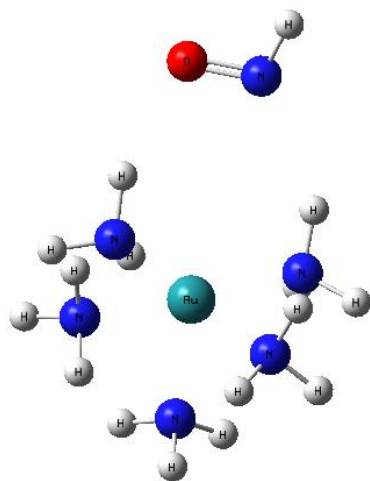
PC

2 1

Ru	-0.41419200	0.00140400	-0.05454400
N	0.70229500	-1.43275500	1.17158800
H	0.38032600	-2.40144200	1.11396700
H	1.68085500	-1.44336200	0.86632000
N	0.54417900	1.62361800	1.06376200
H	1.52212200	1.67465000	0.75850400
H	0.15098400	2.55500000	0.91157000
N	-1.44805500	1.46744100	-1.32257200
H	-0.82113500	1.84485600	-2.03721400
H	-2.25032500	1.09591900	-1.83593800
N	-1.25186600	-1.63666200	-1.25683300
H	-0.71804800	-1.76804200	-2.11946500
H	-1.24438200	-2.54675500	-0.79089600
N	-2.05753600	-0.05056600	1.28122100
H	-2.11491300	-0.92589300	1.80705200
H	-2.02311700	0.69513100	1.98065900
H	0.72363900	-1.21437500	2.17014500
H	0.57462300	1.50295500	2.07868000
H	-2.96042800	0.05142200	0.81166700
H	-1.80639000	2.28099100	-0.81732000
H	-2.22015400	-1.49939500	-1.55539600
N	3.27919900	0.59853200	-0.45960100
O	3.36973900	-0.61313500	-0.39490200
H	4.01538300	0.95440200	-1.12616000

2 Lower vibrational modes in 28.2543 cm^{-1} and 52.9974 cm^{-1} .

Free Energy = -4855.818936 Hartree



trans-¹[Ru(NH₃)₄(py)HNO]²⁺

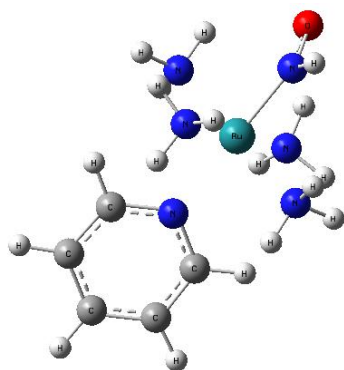
RC

2 1

Ru	-0.81645400	0.01061700	0.11185700
N	-0.91254500	1.41414500	-1.54572100
H	-0.15015000	1.31356000	-2.22000900
H	-1.77799800	1.25999400	-2.07201400
N	-0.68231300	1.58786400	1.63167000
H	-1.34954900	1.48371200	2.39973800
H	0.23682900	1.59929300	2.08038200
N	-0.68920900	-1.42489200	1.76528300
H	-1.26982000	-1.18347600	2.57185200
H	-0.96904300	-2.37704100	1.51800900
N	-0.92633000	-1.55200300	-1.39814400
H	-1.84512900	-1.51436100	-1.85082900
H	-0.23846600	-1.45361200	-2.14841900
H	-0.92847700	2.40410200	-1.28986100
H	-0.83277800	2.53838300	1.28465700
H	0.26048200	-1.50095800	2.13756300
H	-0.83101900	-2.51287200	-1.06034500
N	-2.74108100	0.02249500	0.15036400
O	-3.50434600	-0.06940200	-0.82532500
C	3.50218000	1.18222300	-0.19921000
C	4.20677700	-0.02341400	-0.21587200
C	2.09601300	-1.15835200	-0.03423100
H	4.01041800	2.13880700	-0.26368900
H	5.29008800	-0.03372300	-0.29316500
H	1.51763700	-2.07427900	0.02535500
N	1.40498100	0.00358200	-0.01247700
C	2.11311400	1.15220200	-0.09785600
H	1.55068300	2.07994900	-0.08864200
C	3.48422500	-1.21566000	-0.13280000
H	3.97774400	-2.18200000	-0.14450500
H	-3.28106400	0.12224800	1.03781600

2 Lower vibrational modes in 58.6556 cm⁻¹ and 65.3751 cm⁻¹.

Free Energy = -5047.560643 Hartree



trans-¹[Ru(NH₃)₄(py)HNO]²⁺

TS

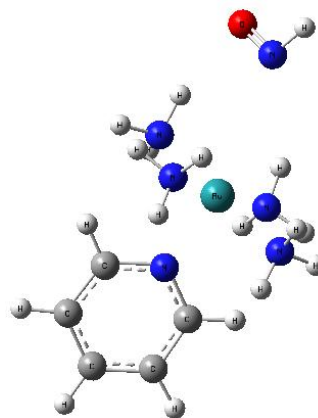
2 1

Ru	-0.58310200	0.25098600	0.15947300
N	-0.66038600	1.34410400	-1.73978200
N	-0.20441700	2.08470900	1.30807600
N	-0.68465500	-0.81895800	2.07416000
N	-1.10601700	-1.54862300	-0.97084200
H	0.02763400	1.03598700	-2.43127600
H	-1.57079600	1.21397700	-2.18783800
H	-0.54439700	2.35793300	-1.67116000
H	-0.89788300	2.20146100	2.05078100
H	0.70193100	2.09388600	1.78186500
H	-0.24512500	2.95508700	0.77243400
H	0.15866500	-0.73668900	2.64729900
H	-1.44148200	-0.44109500	2.64954700
H	-0.87911900	-1.82120600	2.01370100
H	-0.95325100	-2.44214400	-0.49778600
H	-2.10592200	-1.53884300	-1.20074400
H	-0.61291100	-1.63049400	-1.86292900
N	1.43871000	-0.08915000	-0.04203300
C	2.27980600	0.90146600	-0.43020200
C	3.65129600	0.71430900	-0.57671700
C	4.20180500	-0.54236300	-0.31576000
C	3.34165200	-1.56724500	0.08545800
C	1.98019600	-1.30585600	0.21036000
H	1.83553100	1.86938600	-0.62784400
H	4.26647900	1.55121600	-0.89121700
H	5.26831500	-0.71743500	-0.42116800
H	3.70904300	-2.56491500	0.30319800
H	1.29769500	-2.08688000	0.52167600
N	-3.98586200	-0.08360600	-0.03357300
O	-4.22104800	-1.00665800	-0.78938200
H	-4.89967800	0.28945400	0.33883100

2 Lower vibrational modes in 35.3229 cm⁻¹ and 41.1837 cm⁻¹.

1 Imaginary frequency in -147.3394 cm⁻¹.

Free Energy = -5047.511324 Hartree



$trans\text{-}^1[\text{Ru}(\text{NH}_3)_4(\text{py})\text{HNO}]^{2+}$

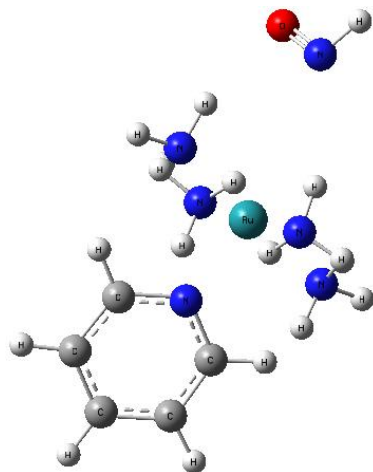
PC

2 1

Ru	-0.57348600	0.24485800	0.19720700
N	-0.73484800	1.19232100	-1.77274600
N	-0.20164700	2.16998500	1.19249500
N	-0.53083600	-0.68625900	2.18345700
N	-1.12531300	-1.64587900	-0.76207700
H	-0.05559400	0.84388500	-2.45360600
H	-1.65107900	1.01834100	-2.19315900
H	-0.63228100	2.20984800	-1.78125700
H	-0.87119700	2.31623800	1.95196600
H	0.72033300	2.24601100	1.62878100
H	-0.29498200	2.99800200	0.59915400
H	0.35949600	-0.56897900	2.67278600
H	-1.23457500	-0.26718500	2.79634300
H	-0.72883100	-1.68906300	2.20652300
H	-0.99665500	-2.49254700	-0.20284600
H	-2.12466400	-1.62950100	-0.99558900
H	-0.63394600	-1.82563100	-1.64061800
N	1.44287700	-0.08372700	-0.06270500
C	2.26217900	0.89580500	-0.51919400
C	3.63121800	0.71494200	-0.69471800
C	4.20194900	-0.52348400	-0.39279100
C	3.36345400	-1.53832500	0.07442600
C	2.00328500	-1.28431400	0.22461600
H	1.80104300	1.84873500	-0.74942500
H	4.22910600	1.54244400	-1.06281000
H	5.26724700	-0.69279600	-0.51801900
H	3.74674200	-2.52240800	0.32430500
H	1.33642700	-2.05812800	0.58426800
N	-4.12022800	-0.06356600	-0.10310500
O	-4.22500900	-1.01676200	-0.85220200
H	-5.08569500	0.31518600	0.09246200

2 Lower vibrational modes in 38.1694 cm^{-1} and 49.8522 cm^{-1} .

Free Energy = -5047.511443 Hartree

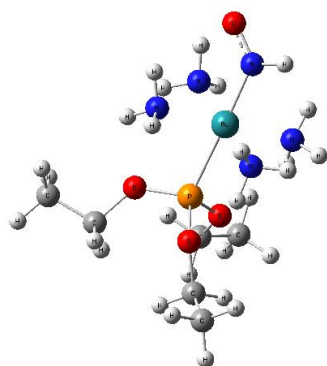


$trans^{-1}[Ru(NH_3)_4(P(OEt)_3)HNO]^{2+}$

RC

2 1			
Ru	1.51486500	0.14669000	0.03169600
N	1.39773900	1.00448800	2.04872400
N	1.40003500	2.15130000	-0.85337200
N	1.59970800	-0.78539700	-1.93401500
N	1.65450800	-1.85703600	0.87515800
H	2.11824600	0.64574000	2.67906900
H	1.49066800	2.02212100	2.08103500
H	0.49995500	0.79588700	2.49492000
H	0.44539800	2.37272500	-1.14970600
H	1.98521700	2.26262100	-1.68470700
H	1.67828600	2.90782200	-0.22412000
H	1.47013700	-0.14379900	-2.71966100
H	2.51029100	-1.23053500	-2.08147100
H	0.89924200	-1.51977200	-2.05957600
H	1.06925200	-2.55259700	0.40707400
H	2.61738700	-2.19817000	0.79586300
H	1.41218400	-1.91962500	1.86661900
P	-0.88174700	0.00777500	-0.01042000
O	-1.38622100	-1.39760900	-0.64371400
O	-1.52376400	0.11294900	1.47609800
O	-1.57305000	1.18633600	-0.88674300
C	-2.60476100	-1.63120700	-1.42949700
C	-2.50063300	-3.00860400	-2.05632700
H	-3.46915000	-1.56592800	-0.76345900
H	-2.67503400	-0.84955300	-2.18971300
H	-3.40332300	-3.20266800	-2.64460600
H	-1.63498100	-3.07209300	-2.72201200
H	-2.41619700	-3.78313200	-1.28865000
C	-2.66990500	-0.63523300	2.00819300
C	-2.63652100	-0.52920800	3.52088600
H	-2.58651100	-1.67296200	1.67713200
H	-3.58564700	-0.19835300	1.60064500
H	-2.70762300	0.51396700	3.84202400
H	-1.71661900	-0.96361500	3.92291500
H	-3.48847300	-1.07684300	3.93667000
C	-2.87362800	1.82108800	-0.63388100
C	-2.95764800	3.07121600	-1.48882200
H	-2.93737300	2.05712500	0.43094300
H	-3.66288600	1.11112700	-0.89412900
H	-3.92522900	3.55525900	-1.32109600
H	-2.16731000	3.78000100	-1.22511800
H	-2.87477400	2.82507700	-2.55132000
N	3.48726000	0.23038000	0.02080100
O	4.27148500	-0.69209600	-0.23221400
H	4.00324200	1.11810900	0.21428800

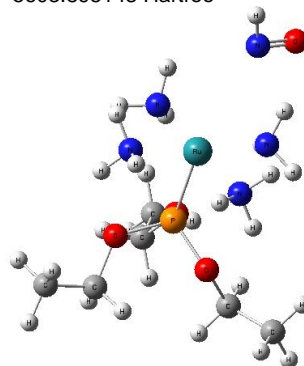
2 Lower vibrational modes in 30.8393 cm^{-1} and 36.2163 cm^{-1} .
Free Energy = -5603.929297 Hartree

 $trans^{-1}[Ru(NH_3)_4(P(OEt)_3)HNO]^{2+}$

TS

2 1			
Ru	-1.27297800	0.38605400	-0.05461800
N	-1.35555700	0.24962200	-2.23639700
N	-0.98841700	2.54696200	-0.14729500
N	-1.31237600	0.50473600	2.13477500
N	-1.78562500	-1.73682500	0.06240000
H	-2.25483700	-0.11828900	-2.55645300
H	-1.23444300	1.13861800	-2.72621900
H	-0.63728600	-0.37125700	-2.61633600
H	-0.06341300	2.83284100	0.18246600
H	-1.67022000	3.04633600	0.42904200
H	-1.07998500	2.94545700	-1.08440400
H	-0.87946100	1.34497400	2.52370800
H	-2.27138300	0.49712700	2.49092000
H	-0.83601400	-0.28004100	2.58394200
H	-1.36428800	-2.23718400	0.84773800
H	-2.80084100	-1.83673100	0.17376100
H	-1.54158100	-2.28088600	-0.76784100
P	0.88959900	-0.00788200	-0.01279600
O	1.29134600	-1.01608200	1.19747800
O	1.47618800	-0.67779800	-1.37189800
O	1.77171500	1.33904900	0.20931600
C	2.54193000	-0.99178900	1.96346600
C	2.39030600	-1.94393200	3.13489500
H	3.36308600	-1.30061700	1.31063500
H	2.71739700	0.03279500	2.30031000
H	3.31542700	-1.94269800	3.72038100
H	1.56906200	-1.63445000	3.78791400
H	2.20257300	-2.96431800	2.78845900
C	2.36186700	-1.84306000	-1.46682700
C	2.18435100	-2.46251800	-2.84046800
H	2.10071100	-2.54697600	-0.67373000
H	3.38998800	-1.50062500	-1.31919100
H	2.42974700	-1.74525200	-3.62904000
H	1.15750200	-2.81144000	-2.98425700
H	2.85740000	-3.32107300	-2.93474500
C	3.10622000	1.61192000	-0.33590700
C	3.34004900	3.10981400	-0.27329900
H	3.14390500	1.24196400	-1.36294000
H	3.84109700	1.07103600	0.26650700
H	4.33997900	3.33297200	-0.65950200
H	2.60714000	3.64638200	-0.88304100
H	3.27965900	3.47340100	0.75664000
N	-4.60094900	0.07998500	0.11129900
O	-4.88546000	-1.09731900	0.21358100
H	-5.49207300	0.64302100	0.07794800

2 Lower vibrational modes in 35.6555 cm^{-1} and 28.0339 cm^{-1} .
1 Imaginary frequency in -63.3199 cm^{-1} .
Free Energy = -5603.895148 Hartree



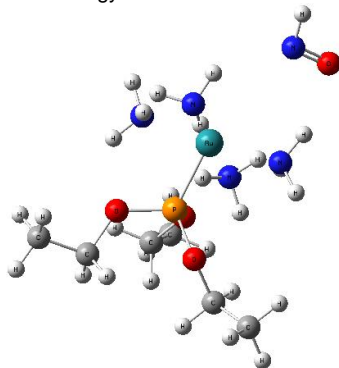
***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺**

PC

2 1

Ru	-1.25004900	0.40947300	0.00636100
N	-1.36557000	0.36894200	-2.17494600
N	-0.96646600	2.57357900	-0.01557900
N	-1.30341600	0.43136800	2.19144800
N	-1.76440000	-1.71852100	0.04430700
H	-2.31738700	0.16484800	-2.48995900
H	-1.10256200	1.24408400	-2.63324500
H	-0.76485600	-0.34474600	-2.59293300
H	0.02137700	2.83380500	0.03817000
H	-1.42938100	3.04182900	0.76683400
H	-1.33459300	3.02533700	-0.85591400
H	-0.93173200	1.28245400	2.61882400
H	-2.26081600	0.33991100	2.54027300
H	-0.77102200	-0.33493400	2.60917200
H	-1.38182000	-2.24228000	0.83408700
H	-2.78560700	-1.79900800	0.11516200
H	-1.49809800	-2.24797300	-0.78852700
P	0.90887100	0.00618100	-0.00577900
O	1.34672100	-0.95852300	1.22602300
O	1.44736200	-0.71107200	-1.36102100
O	1.81556200	1.35078800	0.11976800
C	2.65805500	-0.97550400	1.88291000
C	2.56343600	-1.89536200	3.08567600
H	3.40764200	-1.33480200	1.17234000
H	2.90494700	0.04701900	2.17912700
H	3.53199700	-1.92130800	3.59536700
H	1.81008900	-1.53689100	3.79323000
H	2.30695400	-2.91387100	2.78002700
C	2.22239500	-1.95061900	-1.45705700
C	1.92223300	-2.59618300	-2.79708300
H	1.94686200	-2.60624500	-0.62812300
H	3.28120000	-1.68996500	-1.37005900
H	2.17661200	-1.92408200	-3.62180300
H	0.86481700	-2.86677200	-2.87268400
H	2.52035400	-3.50773800	-2.89840800
C	3.12236400	1.57262000	-0.51127000
C	3.41083000	3.06174700	-0.47689300
H	3.08098400	1.19251500	-1.53419600
H	3.87593500	1.01098000	0.04734100
H	4.39032500	3.24747800	-0.92963500
H	2.65866300	3.61990500	-1.04231500
H	3.43072000	3.43431900	0.55142100
N	-4.81590100	0.10112100	0.07484800
O	-4.90445500	-1.10960500	0.15799100
H	-5.78964000	0.50827700	0.08289000

2 Lower vibrational modes in 19.5071 cm⁻¹ and 27.7343 cm⁻¹.
Free Energy = -5603.898780 Hartree

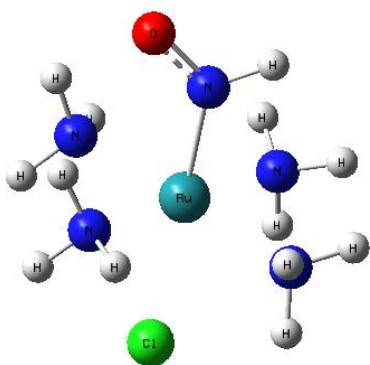




RC

1 1			
Ru	-0.05260700	0.08460700	0.00115500
N	0.45799000	1.57974600	-1.50805700
N	0.49003700	1.53438000	1.54023800
N	-0.44091400	-1.44948600	1.48572300
N	-0.48117300	-1.41690200	-1.50615800
H	1.46414700	1.52067800	-1.68429100
H	-0.00105400	1.45415500	-2.41278800
H	0.27167600	2.54901600	-1.24204300
H	0.40957300	2.51475700	1.26228700
H	-0.02904100	1.45611500	2.41727700
H	1.47537400	1.38529800	1.77210900
H	-0.29100400	-1.14895000	2.45135700
H	-1.40707600	-1.78387200	1.43779900
H	0.16433100	-2.26286600	1.35518500
H	-1.47914300	-1.64573500	-1.52130900
H	-0.23465600	-1.14570000	-2.46040500
H	0.01851200	-2.29150300	-1.33343800
Cl	2.36988200	-0.59315800	-0.02446100
N	-1.89304800	0.56844600	0.02273400
O	-2.88531700	-0.19043000	0.00312500
H	-2.18264000	1.56973900	0.05690600

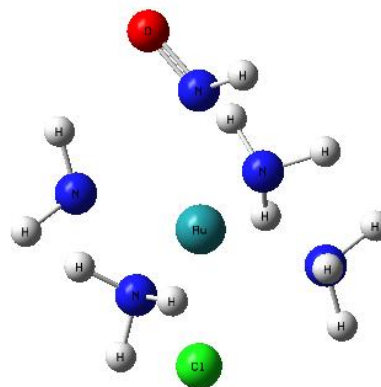
2 Lower vibrational modes in 81.1325 cm⁻¹ and 88.0855 cm⁻¹.
Free Energy = -5259.689389 Hartree



TS

1 1			
Ru	-0.03429800	0.06448100	0.01858300
N	-0.01648400	-0.93586000	1.95814000
N	-0.55329800	1.96477000	0.96039100
N	-0.18981400	1.00475700	-1.94529100
N	0.47801900	-1.83283100	-0.92192300
H	-0.93201100	-1.35999900	2.12637300
H	0.66884400	-1.69049400	2.03241200
H	0.16261500	-0.32384300	2.75674600
H	-0.21528400	2.06983300	1.91922400
H	-0.22336500	2.79605400	0.46504500
H	-1.57182200	2.04873900	1.00866000
H	-0.04947100	2.01684800	-1.94558400
H	0.46342100	0.63905700	-2.64099300
H	-1.12858000	0.84947700	-2.32093900
H	1.48878100	-1.99324200	-0.91681900
H	0.05550600	-2.63860600	-0.45649400
H	0.18321500	-1.89957900	-1.89807600
Cl	-2.41315700	-0.44557500	-0.12836400
N	2.37477300	0.51601200	0.14732500
O	3.27746400	-0.28138200	-0.06970700
H	2.75886700	1.45648200	0.40214300

2 Lower vibrational modes in 20.9541 cm⁻¹ and 89.0222 cm⁻¹.
1 Imaginary frequency in -179.1106 cm⁻¹.
Free Energy = -5259.654791 Hartree

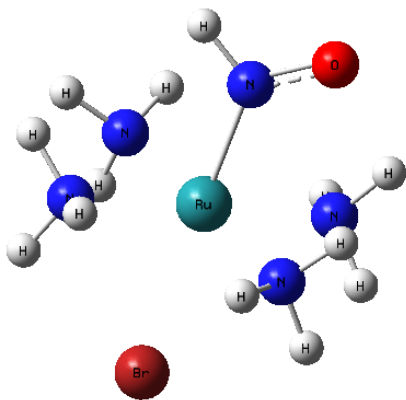


trans-¹[Ru(NH₃)₄(Br)HNO]¹⁺

RC

1 1			
Ru	-0.42043600	0.11646500	-0.00135700
N	-0.61605100	-1.41705600	-1.52546800
N	-0.12342800	1.69109900	-1.49072700
N	-0.12023800	1.61677000	1.56126300
N	-0.62227800	-1.47004800	1.46602300
H	-1.52628400	-1.88220900	-1.46703000
H	-0.53446300	-1.07837000	-2.48656900
H	0.09628700	-2.14361700	-1.42901800
H	-0.60964400	2.57168200	-1.30797600
H	0.87369100	1.91545500	-1.53169800
H	-0.39082300	1.42744500	-2.44144900
H	-0.65953200	1.46036000	2.41553600
H	0.86539600	1.60728400	1.83522100
H	-0.32442400	2.57856600	1.28174400
H	-1.57477300	-1.84579200	1.47299900
H	0.00412700	-2.25473600	1.27581600
H	-0.41929300	-1.18468300	2.42626100
N	-2.31428800	0.33467500	-0.00710800
O	-3.18545300	-0.55859000	0.01249500
H	-2.74447400	1.28492800	-0.03395100
Br	2.21431500	-0.24000400	-0.00222900

2 Lower vibrational modes in 77.4797 cm⁻¹ and 95.9050 cm⁻¹.
Free Energy = -7373.218464 Hartree

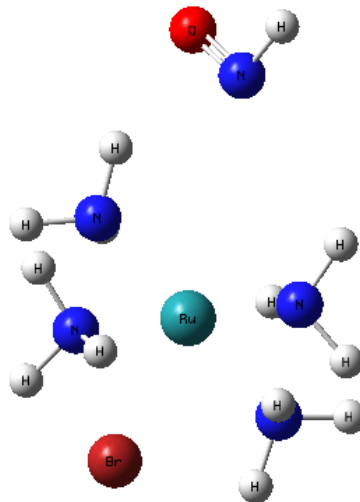


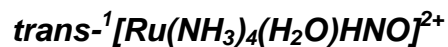
trans-¹[Ru(NH₃)₄(Br)HNO]¹⁺

TS

1 1			
Ru	0.17285400	0.28710000	0.00340600
N	0.27995300	0.05486300	2.17742100
N	-0.58256900	2.33152500	0.23611100
N	0.08015100	0.50910900	-2.17573900
N	0.94890700	-1.74127600	-0.23970200
H	0.00372600	-0.87892800	2.48739300
H	1.21866300	0.20899000	2.55235200
H	-0.33227800	0.69556800	2.68660200
H	-0.17269300	3.00707900	-0.41270100
H	-1.59167500	2.35510800	0.07108200
H	-0.44326100	2.73234200	1.16615600
H	0.83249300	0.03252800	-2.67752500
H	-0.79412300	0.11514300	-2.53175100
H	0.10381100	1.47681600	-2.50373000
H	1.97091500	-1.76803200	-0.16444300
H	0.58991700	-2.39739900	0.45648200
H	0.71763800	-2.15711200	-1.14419900
N	3.75265500	0.32648500	-0.00476200
O	4.01661100	-0.86125800	-0.02603100
H	4.65701100	0.86788900	0.05755100
Br	-2.22435100	-0.58277900	0.00176700

2 Lower vibrational modes in 27.0968 cm⁻¹ and 57.1753 cm⁻¹.
1 Imaginary frequency in -84.0363 cm⁻¹.
Free Energy = -7373.158241 Hartree

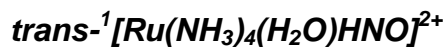
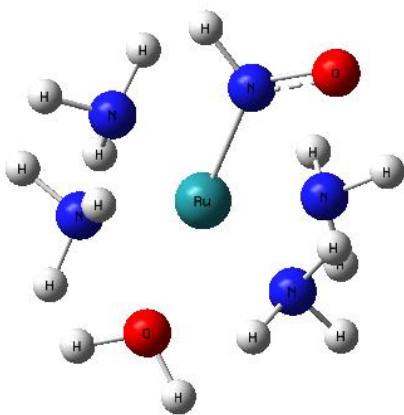




RC

2 1			
Ru	-0.12053100	0.00658300	-0.01233900
N	0.49293500	-1.85438100	0.92299600
N	0.75623900	1.07409700	1.66797200
N	-0.83041900	1.90046600	-0.84134900
N	-1.06901800	-1.09965800	-1.64498800
H	0.01800600	-2.02720500	1.81221400
H	0.32016300	-2.68634800	0.35430400
H	1.49628800	-1.85909600	1.12567800
H	1.74960400	1.24956100	1.49119900
H	0.33364600	1.98658800	1.85424700
H	0.72049000	0.56876200	2.55639800
H	-1.15955700	1.85355900	-1.80829400
H	-1.61654800	2.27097600	-0.30133300
H	-0.12095300	2.63699800	-0.83259100
H	-0.45509800	-1.76620000	-2.11935800
H	-1.85455200	-1.65320200	-1.29311500
H	-1.45843100	-0.51587200	-2.38875600
O	-2.09299400	-0.21628300	1.04908400
H	-2.17374500	-0.05372800	2.00559000
H	-2.92954300	0.08398300	0.65172200
N	1.53711400	0.11475000	-0.90959700
O	2.67542300	0.01597300	-0.42291900
H	1.56618200	0.27712100	-1.93956900

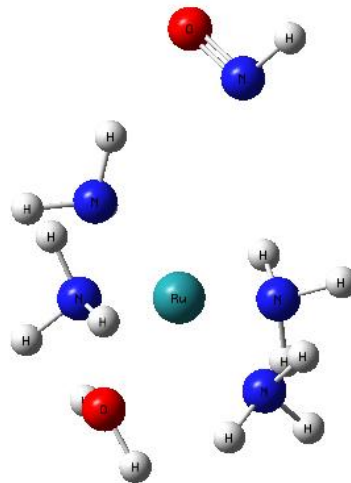
2 Lower vibrational modes in 55.3482 cm^{-1} and 108.4094 cm^{-1} .
Free Energy = -4875.745213 Hartree



TS

2 1			
Ru	0.37295300	0.01346900	0.04893700
N	0.45290000	-2.12063300	0.48375100
N	-0.91899400	-0.40423200	-1.66484900
N	0.32901700	2.15874800	-0.40902300
N	1.62018000	0.41581400	1.81112700
H	1.13145900	-2.58519900	-0.12453200
H	0.73722100	-2.34288100	1.44025700
H	-0.43414600	-2.60896300	0.34312600
H	-1.90496900	-0.41620300	-1.38263400
H	-0.85814800	0.27884200	-2.42358300
H	-0.74040800	-1.31060900	-2.10320100
H	-0.00542000	2.71293600	0.38273200
H	1.24350500	2.54718100	-0.65106800
H	-0.28533900	2.40343300	-1.18864600
H	1.04799900	0.46454000	2.65763600
H	2.32843200	-0.29684100	2.00190800
H	2.12822300	1.30237500	1.77479300
O	2.12533000	-0.31505100	-1.16673300
H	2.05165800	0.01317700	-2.08184500
H	2.94100300	0.08567100	-0.81382200
N	-2.95465300	0.23219200	0.92375900
O	-3.60981500	-0.09392300	-0.04737800
H	-3.61430300	0.45848300	1.71520100

2 Lower vibrational modes in 26.0720 cm^{-1} and 60.1029 cm^{-1} .
1 Imaginary frequency in -160.5666 cm^{-1} .
Free Energy = -4875.679065 Hartree



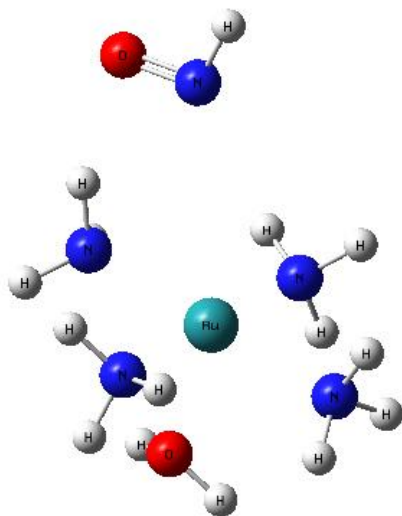
trans-¹[Ru(NH₃)₄(H₂O)HNO]²⁺

PC

2 1

Ru	0.38963600	0.01457700	0.05212200
N	0.45217000	-2.12921800	0.43953100
N	-0.92738900	-0.34454300	-1.65376900
N	0.37216200	2.17078100	-0.35659500
N	1.65324200	0.36580900	1.81245100
H	1.19789100	-2.56760100	-0.10655800
H	0.63811800	-2.37299900	1.41475500
H	-0.40627500	-2.62733900	0.19419300
H	-1.90741300	-0.37081900	-1.35122400
H	-0.88370000	0.36830900	-2.38580100
H	-0.75589200	-1.23175700	-2.13241900
H	0.10418900	2.71733900	0.46524000
H	1.27964500	2.54069900	-0.64899800
H	-0.28374800	2.44810600	-1.09004300
H	1.08428000	0.43550300	2.65969300
H	2.33424300	-0.37328000	2.00163300
H	2.19410700	1.23277900	1.77669600
O	2.12990500	-0.31558600	-1.17845300
H	2.05121800	0.01499300	-2.09226400
H	2.95482900	0.07204000	-0.83267500
N	-3.08802200	0.21855100	0.94321900
O	-3.64978400	-0.09927300	-0.08825800
H	-3.82159000	0.42186500	1.67423000

2 Lower vibrational modes in 28.5357 cm⁻¹ and 65.4357 cm⁻¹.
Free Energy = -4875.679556 Hartree



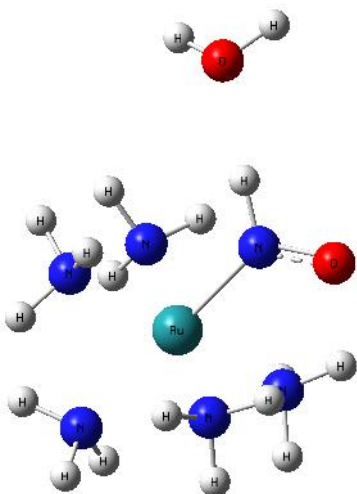
**HNO substitution reactions stationary structures and Free Energies:
B3LYP/DGDZVP SCRF(IEFPCM,SOLVENT=WATER)**



RC

2 1			
Ru	-0.42357900	-0.06304400	0.00242000
N	-1.14634300	1.32205600	-1.51104100
H	-2.10541700	1.64793500	-1.37186500
H	-0.55994700	2.16215000	-1.50725000
N	0.21095800	-1.48017300	-1.54717300
H	0.80451300	-1.05771200	-2.26465800
H	0.74148400	-2.27950700	-1.19387200
N	0.26970900	-1.44489000	1.55990100
H	0.75388000	-0.97007400	2.32512600
H	-0.49354900	-1.96355800	2.00074000
N	-1.11364100	1.34692400	1.50981400
H	-0.44647800	2.12098900	1.58120000
H	-2.01768400	1.77885800	1.30575900
N	-2.41747500	-1.12654100	0.02795400
H	-3.00505700	-0.89134900	-0.77516000
H	-2.34769600	-2.14671800	0.02084100
H	-1.11557400	0.96142500	-2.46746000
H	-0.58057400	-1.88449100	-2.05289700
H	-2.98352100	-0.89941700	0.84875100
H	0.92555300	-2.15605200	1.22860600
H	-1.20144400	0.95973400	2.45237200
N	1.26145400	0.84275400	-0.02235000
O	1.44743000	2.07678300	-0.02094000
H	2.17286400	0.31553900	-0.03466700
O	3.83760500	-0.53262700	-0.10156500
H	3.84003600	-1.43622100	0.25648300
H	4.52315700	-0.06175800	0.40178100

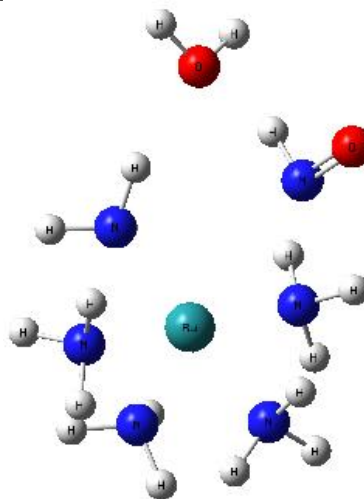
2 Lower vibrational modes in 43.7695 cm^{-1} and 61.9260 cm^{-1} .
Free Energy = -4932.304053 Hartree



TSI

2 1			
Ru	-0.66457500	-0.04098400	0.00528600
N	-0.88622000	-0.19574800	2.18145700
H	-1.51335700	-0.94101300	2.49250300
H	0.01302200	-0.39361100	2.62681100
N	-0.24615600	2.09707800	0.19605900
H	0.77242600	2.24559900	0.17564600
H	-0.63391700	2.67581500	-0.55227700
N	-0.33777500	0.09506500	-2.16089400
H	0.39062600	-0.55230100	-2.47099200
H	-1.15662200	-0.12453400	-2.73286500
N	-0.96275700	-2.20583300	-0.18868300
H	-0.07510000	-2.69492600	-0.04979600
H	-1.61048400	-2.61914500	0.48588400
N	-2.74008300	0.33713400	-0.21441800
H	-3.14609600	0.79028500	0.60774700
H	-2.95899400	0.95064300	-1.00309300
H	-1.23181400	0.65185100	2.63739300
H	-0.57958500	2.52258500	1.06355300
H	-3.28945200	-0.51288000	-0.36333100
H	-0.02971200	1.01866900	-2.47264600
H	-1.30009000	-2.50590100	-1.10610500
N	2.76944300	-1.05221100	0.12685900
O	3.81859400	-1.67236600	0.06580600
H	2.97899500	-0.01860000	0.08991000
O	2.80282800	2.03513000	0.03349900
H	3.16500600	2.41212300	-0.78641200
H	3.29991200	2.46814300	0.74839100

2 Lower vibrational modes in 29.7197 cm^{-1} and 43.5671 cm^{-1} .
1 Imaginary frequency in -20.9441 cm^{-1} .
Free Energy = -4932.249516 Hartree

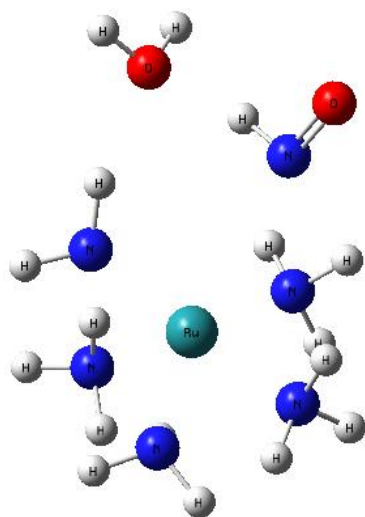




INT

2 1			
Ru	-0.66266000	-0.04394000	0.00775100
N	-0.89739900	-0.16210900	2.18564100
H	-1.51599300	-0.91040200	2.50652100
H	0.00066600	-0.33675600	2.64294300
N	-0.35993600	2.11346200	0.15375500
H	0.65229300	2.30075100	0.14841800
H	-0.75648900	2.65846400	-0.61501700
N	-0.33371800	0.06238200	-2.16123500
H	0.44240400	-0.53509200	-2.45497800
H	-1.13267000	-0.23416200	-2.72661700
N	-0.78007200	-2.23542200	-0.14223900
H	0.16074500	-2.62164000	-0.02884200
H	-1.35640000	-2.69787900	0.56420500
N	-2.75301600	0.18743900	-0.24578400
H	-3.21015200	0.57372300	0.58343200
H	-3.00018300	0.81491600	-1.01482600
H	-1.26020100	0.68961800	2.62028500
H	-0.72817600	2.54449700	1.00433100
H	-3.23046000	-0.69572400	-0.44162900
H	-0.09686500	0.99824700	-2.49779600
H	-1.11702900	-2.58702300	-1.04125700
N	2.78420300	-1.03115500	0.14540000
O	3.89741100	-1.52421400	0.05898100
H	2.87672300	0.02014100	0.11922900
O	2.67802300	2.07822900	0.03775500
H	3.04391600	2.44854700	-0.78359000
H	3.16104300	2.52883300	0.75146600

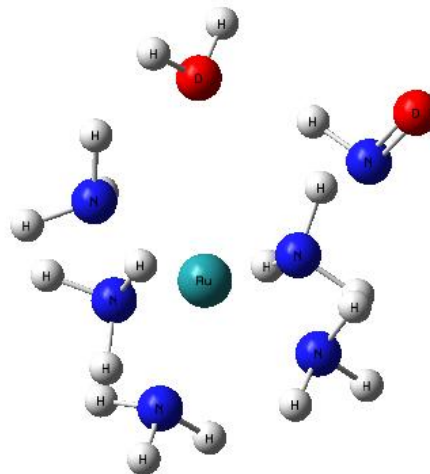
2 Lower vibrational modes in 21.9396 cm^{-1} and 48.1023 cm^{-1} .
Free Energy = -4932.250191 Hartree



TSII

2 1			
Ru	0.62136400	-0.07163500	0.00295400
N	0.32482300	0.25526700	-2.14642300
H	0.69864100	-0.47788200	-2.75373700
H	-0.67160100	0.30766500	-2.37016600
N	1.53205900	1.90499700	0.19127800
H	0.75667300	2.57361400	0.20780700
H	2.06668500	2.06585300	1.04763000
N	0.82979800	-0.36428300	2.16940200
H	0.15144400	0.20046700	2.68601800
H	0.67857500	-1.32496800	2.48545700
N	-0.40059000	-2.01094200	-0.18487800
H	-1.41510200	-1.87807700	-0.09843800
H	-0.25378700	-2.47571500	-1.08332100
N	2.49671400	-1.00290300	-0.31704800
H	3.26635600	-0.32974900	-0.34090800
H	2.73791500	-1.67685000	0.41354200
H	0.72805400	1.12644100	-2.49797400
H	2.14778000	2.19648400	-0.57147400
H	2.55244200	-1.52030300	-1.19763200
H	1.74415600	-0.09934500	2.54315400
H	-0.14250500	-2.70347000	0.52121900
N	-3.18736000	-0.49249700	0.04436500
O	-4.40329900	-0.44840900	0.10969700
H	-2.80034100	0.48952700	0.05884200
O	-1.49864000	2.11883400	0.15874700
H	-1.78115400	2.59484700	0.95860900
H	-1.75685100	2.69251100	-0.58304600

2 Lower vibrational modes in 27.7778 cm^{-1} and 54.0471 cm^{-1} .
1 Imaginary frequency in -116.2609 cm^{-1} .
Free Energy = -4932.246345 Hartree



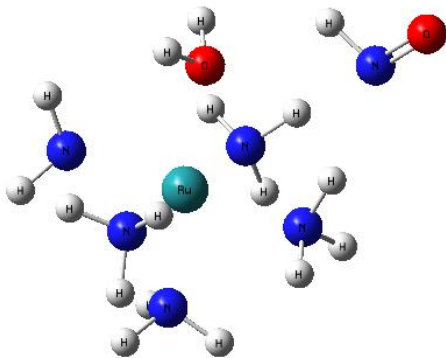


PC

2 1

Ru	-0.66726700	-0.01112700	0.00318500
N	-0.71243100	0.59243600	2.11881600
H	-1.23306400	-0.04711500	2.72397200
H	0.22040500	0.64548700	2.53487100
N	-2.17275100	1.52407500	-0.47081200
H	-1.77751400	2.46314300	-0.56009700
H	-2.67336400	1.35804500	-1.34708300
N	-0.56237800	-0.61401600	-2.11012000
H	-0.99101500	0.05031400	-2.75857700
H	0.40028800	-0.72506500	-2.43731700
N	0.84486900	-1.52353800	0.48056000
H	1.79908100	-1.16341000	0.36112900
H	0.79400700	-1.86252400	1.44400100
N	-2.24269600	-1.44389700	0.35115700
H	-2.94175600	-1.46489900	-0.39536800
H	-1.90505800	-2.40567200	0.43593600
H	-1.13048300	1.51196600	2.27777800
H	-2.90308900	1.60475400	0.24032100
H	-2.77304200	-1.26670800	1.20737400
H	-1.01528800	-1.50985600	-2.30504000
H	0.79297200	-2.36182800	-0.10286400
N	3.69325800	-0.04473600	-0.02451200
O	4.90520500	-0.05396200	0.06272900
H	3.37176800	0.89602100	-0.37735100
O	1.01483000	1.46074200	-0.37402000
H	0.98515000	1.87162400	-1.25632800
H	1.04435300	2.20880200	0.24922200

2 Lower vibrational modes in 55.6446 cm^{-1} and 71.2222 cm^{-1} .
Free Energy = -4932.258230 Hartree

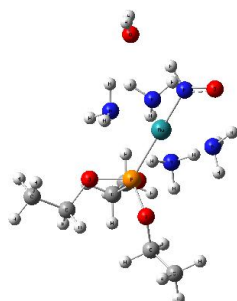


***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺ + H₂O**

RC

2 1			
Ru	-1.27427400	-0.28079900	0.04114000
N	-1.56328600	1.66902700	-0.91443400
N	-1.34777200	0.69545300	2.00325800
N	-1.08121800	-2.23333900	1.00237600
N	-1.11764600	-1.32620700	-1.86601600
H	-1.56887100	1.62074900	-1.93559700
H	-2.45583500	2.10671900	-0.65209800
H	-0.81912000	2.33105200	-0.68416500
H	-0.46112100	0.60357200	2.50569500
H	-2.06397000	0.30640800	2.62000300
H	-1.53749900	1.69880300	1.95582300
H	-0.84343000	-2.20249900	1.99608700
H	-1.98154100	-2.71846400	0.93974400
H	-0.39328800	-2.85769000	0.57595700
H	-0.22172000	-1.80857200	-1.97501700
H	-1.84515300	-2.04128000	-1.95183800
H	-1.21422200	-0.73423200	-2.69411600
P	1.10454700	0.06470100	0.00246400
O	1.85850700	-1.07162500	-0.88057600
O	1.54166400	1.49432600	-0.63263800
O	1.75850700	0.02181700	1.48994800
C	3.16553500	-1.68499600	-0.62259300
C	3.26103000	-2.95009600	-1.45445400
H	3.94555900	-0.97031900	-0.89857500
H	3.23805400	-1.90322200	0.44559500
H	4.23359200	-3.42170900	-1.28014300
H	2.47702900	-3.66022600	-1.17571900
H	3.17342900	-2.72473000	-2.52125400
C	2.70197200	1.76717200	-1.48664500
C	2.48090300	3.10723500	-2.16291800
H	2.78990800	0.95990300	-2.21774400
H	3.59836100	1.78355900	-0.86049400
H	2.37975300	3.90700600	-1.42350000
H	1.58337600	3.08593700	-2.78786500
H	3.34157200	3.33396700	-2.80051600
C	2.93572100	0.77112800	1.94832500
C	2.99456800	0.67530300	3.46113700
H	2.83325700	1.80688000	1.61604200
H	3.82741400	0.33360100	1.49152700
H	3.87604900	1.21684300	3.81946200
H	2.10709600	1.12251300	3.91839100
H	3.07487200	-0.36633900	3.78512900
N	-3.22634000	-0.56055900	-0.00266500
O	-3.83552700	-1.63527600	-0.09444600
H	-3.87933300	0.26241000	0.01325700
O	-4.42098800	2.13478800	-0.05718100
H	-5.10773000	2.37632800	-0.70204600
H	-4.68849500	2.56033900	0.77526500

2 Lower vibrational modes in 17.6490 cm⁻¹ and 30.6561 cm⁻¹.
Free Energy = -5680.365010 Hartree

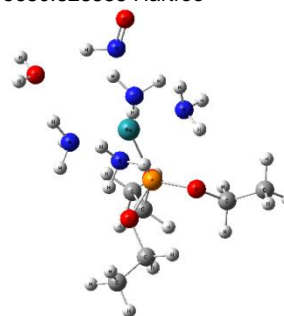


***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺ + H₂O**

TSI

2 1			
Ru	1.05182400	0.03725900	0.00227100
N	1.23940800	-2.12426900	0.21403000
N	1.11308200	0.22259100	2.18659000
N	1.17249500	2.19981900	-0.21973500
N	1.11282000	-0.21835400	-2.16998500
H	0.78611500	-2.67538400	-0.51738300
H	2.24578200	-2.34159000	0.16887400
H	0.89885600	-2.51082200	1.09661400
H	1.16265400	1.18294700	2.53268300
H	1.92844800	-0.25274400	2.58075600
H	0.29152400	-0.18975300	2.63499000
H	0.87259900	2.73234500	0.59938500
H	2.15144900	2.45083600	-0.38122500
H	0.63463000	2.58490600	-0.99852700
H	0.44069100	-0.91195900	-2.50514400
H	0.92198700	0.63021200	-2.70667900
H	2.03340100	-0.54003600	-2.47945700
P	-1.14271300	0.02328000	-0.01883500
O	-1.74108000	-1.07792600	-1.05534600
O	-1.78850400	-0.31194800	1.43392500
O	-1.80677100	1.43226200	-0.47727700
C	-2.99072000	-0.94749600	-1.81318800
C	-3.01226200	-2.03282700	-2.87307200
H	-3.83203800	-1.05630400	-1.12324700
H	-3.02134600	0.04961500	-2.25840900
H	-3.94291200	-1.95639600	-3.44479500
H	-2.17271300	-1.92233400	-3.56581400
H	-2.96809400	-3.02668800	-2.41831200
C	-2.96879900	-1.13515300	1.70944900
C	-2.91569300	-1.55742400	3.16602400
H	-2.95263400	-2.00090600	1.04325700
H	-3.86268700	-0.53905100	1.50452800
H	-2.91815300	-0.68590300	3.82715000
H	-2.02050500	-2.15329400	3.36712800
H	-3.79606300	-2.16658100	3.39561200
C	-2.95864700	2.10176800	0.13144600
C	-2.87356400	3.57994900	-0.20218100
H	-2.93247200	1.93411000	1.21049600
H	-3.86990800	1.65602400	-0.27816500
H	-3.73567700	4.09703900	0.23187500
H	-1.96151600	4.02148100	0.21025400
H	-2.88573800	3.73881300	-1.28442100
N	4.26566400	0.90875300	-0.06539100
O	5.23500600	1.64659700	-0.05211900
H	4.58452100	-0.09684000	-0.02529700
O	4.27569200	-2.16754300	0.06533400
H	4.64749000	-2.62400800	-0.70871600
H	4.73185400	-2.56053800	0.82902800

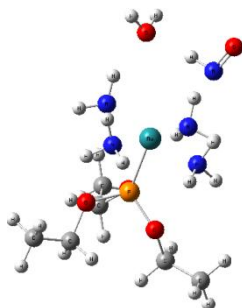
2 Lower vibrational modes in 19.2476 and 28.0850 cm⁻¹.
1 Imaginary frequency in -50.0432 cm⁻¹.
Free Energy = -5680.328558 Hartree



***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺ + H₂O
INT**

2 1			
Ru	-1.02539000	-0.02207600	0.13369000
N	-1.07894100	-2.19327700	-0.03525000
N	-1.24308500	0.09450500	-2.03661900
N	-1.32709000	2.13068200	0.29227700
N	-0.97756400	-0.20483400	2.31482800
H	-0.69235900	-2.71459200	0.75368900
H	-2.07827700	-2.43521900	-0.09199000
H	-0.63350900	-2.58360700	-0.86810000
H	-1.21549300	1.04131300	-2.42083300
H	-2.13836400	-0.29884400	-2.33759600
H	-0.52009000	-0.42541100	-2.53953500
H	-0.88988200	2.68476000	-0.44653900
H	-2.33743900	2.30042200	0.23288100
H	-1.01351000	2.55442900	1.16763100
H	-0.20430500	-0.78853900	2.64125800
H	-0.87674200	0.68232300	2.81194500
H	-1.83460400	-0.63030500	2.67689300
P	1.16156400	0.06005100	0.00902200
O	1.88269500	-0.70335700	1.25080700
O	1.71622300	-0.65920400	-1.34131300
O	1.79228800	1.55560200	-0.00625100
C	3.16498100	-0.34389500	1.86354100
C	3.25059600	-1.03791500	3.21033900
H	3.97059800	-0.67099400	1.20029600
H	3.20706100	0.74253100	1.97021900
H	4.20999400	-0.79604300	3.67919400
H	2.44834600	-0.70363500	3.87483300
H	3.18708300	-2.12400900	3.09622900
C	2.91447900	-1.49351400	-1.45697600
C	2.80458700	-2.29470100	-2.74100400
H	2.96891200	-2.14786400	-0.58376200
H	3.79256400	-0.84116100	-1.47157100
H	2.73409800	-1.63442200	-3.61031200
H	1.92640800	-2.94688300	-2.71864500
H	3.69694600	-2.91907700	-2.85334000
C	2.90376200	2.02668100	-0.83656700
C	2.80746900	3.53774700	-0.93938500
H	2.83216900	1.55459700	-1.81910000
H	3.84144000	1.72368100	-0.36142100
H	3.64012400	3.91016900	-1.54525200
H	1.87033200	3.83819500	-1.41722000
H	2.86607500	4.00295900	0.04896700
N	-4.47874500	1.05478600	0.01458900
O	-5.65881200	1.35643700	-0.04433700
H	-4.39160300	0.00608400	-0.08108600
O	-4.09810700	-2.04689400	-0.21899000
H	-4.60594700	-2.49536900	0.47885600
H	-4.47791400	-2.37503000	-1.05207600

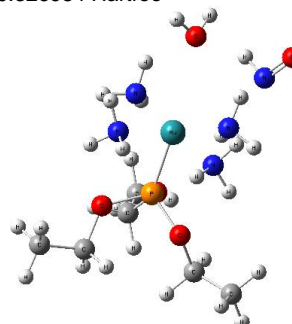
2 Lower vibrational modes in 21.6239 cm⁻¹ and 26.2983 cm⁻¹.
Free Energy = -5680.328800 Hartree



***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺ + H₂O
TSII**

2 1			
Ru	-1.01643700	-0.37665100	0.16576200
N	-0.74037900	-2.44379000	-0.46075800
N	-1.34707100	0.17057500	-1.92702900
N	-1.50953400	1.66066900	0.77573300
N	-0.83416800	-1.00150500	2.25456100
H	-0.29239900	-3.05722600	0.22262300
H	-1.67908500	-2.82046400	-0.62156300
H	-0.21749100	-2.56992100	-1.32945300
H	-1.37930900	1.17690300	-2.10323200
H	-2.24442500	-0.19623900	-2.25313300
H	-0.64165200	-0.19583300	-2.57038200
H	-0.96032200	2.36846400	0.28414100
H	-2.50022100	1.85715000	0.58651200
H	-1.36813600	1.85475900	1.76907000
H	0.05464000	-1.46938900	2.44515000
H	-0.88953800	-0.24015000	2.93442000
H	-1.57098600	-1.66051700	2.51811000
P	1.12535000	0.07786500	0.01451800
O	2.02442100	-0.60126700	1.18628000
O	1.74881300	-0.45994400	-1.38839300
O	1.46159600	1.66740400	0.06811900
C	3.20247400	-0.00693300	1.82589700
C	3.49291500	-0.78889100	3.09329100
H	4.04221700	-0.06382200	1.12763200
H	2.98717400	1.04177900	2.04379700
H	4.37624800	-0.36448300	3.58149800
H	2.65198700	-0.73041400	3.79054500
C	3.69528700	-1.84006800	2.86835000
H	3.09462400	-1.00380300	-1.59210800
C	3.11739100	-1.70557400	-2.93735900
H	3.31526600	-1.69620500	-0.77622900
H	3.81347500	-0.17973000	-1.56755600
H	2.88430000	-1.00824400	-3.74730100
H	2.39809700	-2.52950400	-2.96129500
H	4.11783600	-2.11473300	-3.11196000
C	2.47120800	2.37676600	-0.72230500
C	2.11558600	3.85210800	-0.72267400
H	2.47364600	1.96708900	-1.73500600
H	3.44989800	2.20766500	-0.26396500
H	2.86774300	4.40275400	-1.29707000
H	1.13803300	4.01898400	-1.18474700
H	2.09949800	4.25158400	0.29552100
N	-4.59748000	1.20561700	0.08384500
O	-5.74940700	1.58640800	-0.02409400
H	-4.54732500	0.17147100	-0.12300700
O	-3.70856500	-1.73217500	-0.37673200
H	-4.06959400	-2.25071700	0.36293000
H	-4.14153000	-2.09267400	-1.17006700

2 Lower vibrational modes in 20.4384 cm⁻¹ and 22.6360 cm⁻¹.
1 Imaginary frequency in -47.4859 cm⁻¹.
Free Energy = -5680.326984 Hartree

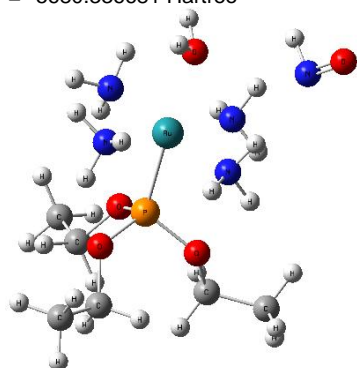


***trans*⁻¹[Ru(NH₃)₄(P(OEt)₃)HNO]²⁺ + H₂O**
PC

2 1

Ru	-0.98978700	-0.67778200	-0.00238400
N	-0.35127500	-2.62901400	-0.78826900
N	-1.32165000	0.03121300	-2.04475400
N	-1.76170900	1.23291000	0.72047500
N	-0.81353800	-1.39938700	2.06057800
H	-0.26038700	-3.35904000	-0.07840900
H	-0.98781600	-3.01210200	-1.49106700
H	0.56334100	-2.57308500	-1.24332400
H	-1.04730300	1.00485400	-2.19132200
H	-2.31321400	-0.01745800	-2.29219900
H	-0.82869500	-0.50061900	-2.76497600
H	-1.31239700	2.03896500	0.27956800
H	-2.76748200	1.31978900	0.52598800
H	-1.65105200	1.38199100	1.72582500
H	0.10307700	-1.17483800	2.45630500
H	-1.49922300	-0.98449900	2.69610600
H	-0.92676700	-2.41031000	2.16414100
P	1.09994000	0.08652800	0.00914300
O	1.83503900	-0.03227800	1.46154600
O	2.09118000	-0.69048300	-1.02698900
O	1.19237600	1.66060700	-0.39785800
C	2.74649100	0.94565000	2.05743100
C	2.87485300	0.62872700	3.53603300
H	3.71523500	0.87185500	1.55465200
H	2.33626000	1.94597800	1.89861400
H	3.56315400	1.34332800	3.99901800
H	1.90589900	0.70785300	4.03781200
H	3.27136900	-0.37949300	3.68761400
C	3.51815000	-0.94665500	-0.81855900
C	3.99355000	-1.87584100	-1.92015800
H	3.64672500	-1.39667100	0.16896000
H	4.05745900	0.00423600	-0.84964300
H	3.85034300	-1.42153100	-2.90492700
H	3.45627200	-2.82835700	-1.88779300
H	5.06113400	-2.07760400	-1.78505500
C	2.26219900	2.31442200	-1.15276300
C	1.74121300	3.65586000	-1.63535400
H	2.54042000	1.67085600	-1.99091600
H	3.12790900	2.44206900	-0.49622000
H	2.52652800	4.16536100	-2.20317500
H	0.87261000	3.52389400	-2.28730800
H	1.45726400	4.29208800	-0.79196800
N	-4.88844700	1.17034400	-0.09055500
O	-5.94882900	1.72803000	0.10896300
H	-5.05776000	0.27331600	-0.61973600
O	-3.19888700	-1.38305100	-0.01845900
H	-3.55429200	-1.64788900	0.84845400
H	-3.42652400	-2.11648000	-0.61699000

2 Lower vibrational modes in 8.9626 cm⁻¹ and 26.2410 cm⁻¹.
 Free Energy = -5680.336681 Hartree

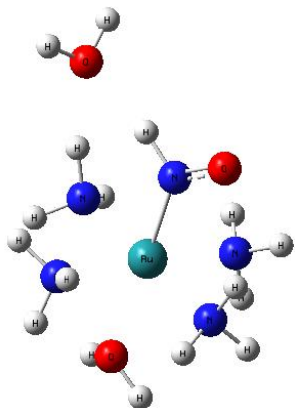


***trans*⁻¹[Ru(NH₃)₄(H₂O)HNO]²⁺ + H₂O**

RC

2 1			
Ru	-0.37394600	-0.06579700	0.00939500
N	-0.23205100	-0.77302500	-2.04311300
N	0.93067400	-1.71295300	0.63574300
N	-0.74014400	0.51796500	2.07330600
N	-1.68508500	1.55660500	-0.63141100
H	-0.25109700	-0.03606300	-2.75135700
H	0.60155000	-1.32878400	-2.24619400
H	-1.03344300	-1.37982000	-2.23627700
H	1.93054300	-1.50123700	0.51917700
H	0.81141400	-1.97455600	1.61705400
H	0.76639300	-2.57384800	0.10863200
H	-0.74537600	1.53269800	2.20174000
H	-1.64948200	0.18610800	2.40407100
H	-0.05311200	0.16075100	2.74080400
H	-1.12722200	2.40750900	-0.74500200
H	-2.15511800	1.39795700	-1.52544700
H	-2.42965200	1.79135800	0.02926300
O	-2.14062200	-1.47931100	0.08891200
H	-2.08679700	-2.30563400	0.60090300
H	-3.03516100	-1.12741200	0.24265300
N	1.11441500	1.09478800	-0.12084000
O	1.12877200	2.33806300	-0.15862200
H	2.08023100	0.68437300	-0.15219400
O	3.60428200	-0.47229000	0.00934200
H	4.27813400	-0.23002300	0.66742900
H	4.09770200	-0.68364900	-0.80149900

2 Lower vibrational modes in 38.0939 cm⁻¹ and 83.3522 cm⁻¹.
Free Energy = -4952.180141 Hartree

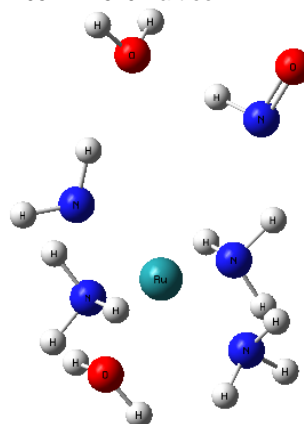


***trans*⁻¹[Ru(NH₃)₄(H₂O)HNO]²⁺ + H₂O**

TSI

2 1			
Ru	0.69315600	-0.05894000	0.01370600
N	0.58459200	0.00674200	-2.16354900
N	0.19867700	2.06619300	0.08281900
N	0.84217400	-0.12780300	2.20047700
N	1.10381800	-2.21111300	-0.08131700
H	0.35908100	-0.88960300	-2.60042100
H	-0.10323700	0.66891800	-2.52862600
H	1.48560900	0.29126500	-2.55552700
H	-0.82568700	2.17487900	0.07491800
H	0.53095200	2.56639000	0.91048400
H	0.54778400	2.60283600	-0.71463600
H	1.69633200	-0.57389400	2.54255400
H	0.81855100	0.78991900	2.65022600
H	0.07121500	-0.65481400	2.61765600
H	0.25221500	-2.73701900	-0.29232300
H	1.77718600	-2.48045800	-0.80225000
H	1.46174300	-2.61176300	0.78841000
O	2.78167800	0.42087600	-0.22707100
H	3.03651800	1.27645500	0.16468200
H	3.40195300	-0.23099000	0.14797800
N	-2.99650400	-1.12930100	0.01425100
O	-4.17928900	-1.43543500	0.02411300
H	-2.93448600	-0.07585200	0.01831500
O	-2.81456400	1.95653200	0.02609000
H	-3.27905600	2.35524900	0.78184800
H	-3.22743100	2.35305500	-0.76018100

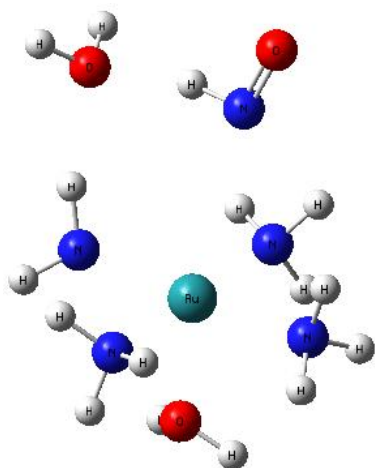
2 Lower vibrational modes in 5.7183 and 20.0146cm⁻¹.
1 Imaginary frequency in -19.1966 cm⁻¹.
Free Energy = -4952.112640 Hartree



***trans*⁻¹[Ru(NH₃)₄(H₂O)HNO]²⁺ + H₂O
INT**

2 1			
Ru	0.65001800	-0.04228500	0.00123400
N	0.95755100	-0.11229800	-2.15429400
N	0.33558200	2.11059200	-0.12071700
N	0.34634700	0.03284100	2.17204400
N	0.79467300	-2.22987100	0.11250900
H	0.78413000	-1.02726800	-2.57602600
H	0.37509300	0.54305800	-2.68029900
H	1.92612500	0.12277600	-2.38468900
H	-0.67898000	2.28723800	-0.12850000
H	0.71398500	2.65387100	0.65844200
H	0.71394600	2.54851100	-0.96340500
H	-0.38991100	-0.60655600	2.47985200
H	1.17607700	-0.22359600	2.71230800
H	0.06908600	0.95361900	2.51870500
H	-0.14039300	-2.62676800	-0.01178400
H	1.38033000	-2.66813300	-0.60193400
H	1.13362300	-2.59422700	1.00559200
O	2.78883000	0.19696900	0.12780800
H	3.09134200	0.95491000	0.66079000
H	3.25856500	-0.57871600	0.48541100
N	-2.79456100	-1.02429000	-0.15681300
O	-3.88125400	-1.57561700	-0.09546500
H	-2.93949600	0.02071500	-0.12779500
O	-2.69733000	2.08585000	-0.04221700
H	-3.07049800	2.46273900	0.77288200
H	-3.16293500	2.54192600	-0.76397700

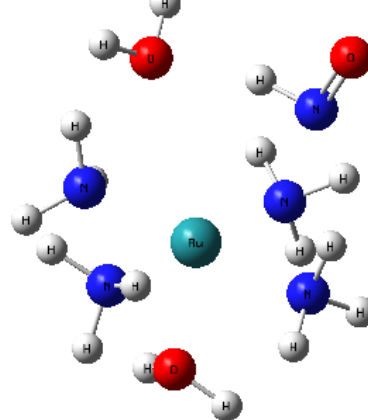
2 Lower vibrational modes in 18.4103 cm⁻¹ and 33.9983 cm⁻¹.
Free Energy = -4952.113304 Hartree



***trans*⁻¹[Ru(NH₃)₄(H₂O)HNO]²⁺ + H₂O
TSII**

2 1			
Ru	0.59890200	-0.06722500	0.01539500
N	0.50216000	0.16309900	-2.14960500
N	1.49946300	1.90873100	0.17801700
N	0.72560200	-0.32261800	2.19249000
N	-0.38171700	-2.02490200	-0.15885300
H	-0.29425600	-0.30972200	-2.58238600
H	0.45037600	1.13220200	-2.47124500
H	1.33749400	-0.23333800	-2.58741500
H	0.72580000	2.57854200	0.21797200
H	2.06953500	2.07202100	1.01080800
H	2.08467500	2.18652000	-0.61286500
H	-0.09448500	-0.79037400	2.58507000
H	1.52846500	-0.88301800	2.48751500
H	0.80346900	0.55884900	2.70471800
H	-1.39999000	-1.89466700	-0.12948600
H	-0.18299700	-2.51990600	-1.03117000
H	-0.15645600	-2.68538900	0.58834300
O	2.51780200	-0.98245000	-0.32331600
H	3.26718700	-0.52510800	0.10055600
H	2.58755900	-1.91457200	-0.04682600
N	-3.16856700	-0.47963700	-0.01585400
O	-4.38454100	-0.46358200	0.05870900
H	-2.80360100	0.51049500	0.00184800
O	-1.50192300	2.14917700	0.08718700
H	-1.81712700	2.64335800	0.86349200
H	-1.74661100	2.69412200	-0.68029100

2 Lower vibrational modes in 28.4909 cm⁻¹ and 40.9733 cm⁻¹.
1 Imaginary frequency in -124.8577 cm⁻¹.
Free Energy = -4952.109254 Hartree



***trans*⁻¹[Ru(NH₃)₄(H₂O)HNO]²⁺ + H₂O**
PC

2 1

Ru	0.65755700	0.00227400	0.00195400
N	0.61697100	-1.46743700	-1.61688800
N	2.19173900	1.15009700	-1.07342500
N	0.73430500	1.43095500	1.66803100
N	-0.88245600	-1.13816900	1.05102700
H	-0.28793100	-1.92476200	-1.75011500
H	0.87724000	-1.10689000	-2.53777400
H	1.28210400	-2.21864400	-1.41651000
H	1.79773400	1.79756200	-1.75997400
H	2.78214600	1.72500500	-0.46809900
H	2.84045900	0.55998400	-1.59935600
H	-0.16467500	1.55932600	2.13851500
H	1.38415500	1.13645000	2.40073400
H	1.03520600	2.37160500	1.40269900
H	-1.82430300	-0.82417900	0.78578300
H	-0.85789600	-2.14259800	0.86040600
H	-0.84043900	-1.05865200	2.06976100
O	2.23111200	-1.25874300	0.89038100
H	3.08404400	-0.82000700	1.05876500
H	1.99716600	-1.69884900	1.72723100
N	-3.71567200	0.09190000	0.08293700
O	-4.89775000	-0.16104200	-0.03477500
H	-3.50122900	0.99941900	-0.41107100
O	-0.97900400	1.15888700	-0.93841700
H	-0.93667500	2.12284600	-0.80358200
H	-1.04867300	1.03808700	-1.90269400

2 Lower vibrational modes in 40.8806 cm⁻¹ and 61.8242 cm⁻¹.
 Free Energy = -4952.123755 Hartree

