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The Role of π–Donor/Acceptor *trans* Effect on The NO release in Ruthenium Nitrosyl Complexes: A Computational Insight

Renato Pereira Orenha,*[a] Nelson Henrique Morgon,[b] Graziele Cappato Guerra Silva,[a] Giovanni Finoto Caramori,[c] and Renato Luis Tame Parreira*[a]

Supplementary Material

[a.] *Núcleo de Pesquisas em Ciências Exatas e Tecnológicas, Universidade de Franca, Franca, SP, Brazil. E–mail: rpo9@hotmail.com / renato.parreira@unifran.edu.br*
[b.] *Instituto de Química, Universidade Estadual de Campinas, CP 6154, 13083–970, Campinas, SP, Brazil.*
[c.] *Departamento de Química, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CP 476, Florianópolis, SC, 88040–900, Brazil.*

Table S1. Optimized Cartesian coordinates, and number of imaginary frequencies (NIMAG) of the structures investigated in this study at PBE0/Def2TZV with PCM(H_2O) solvation.

trans–[RuCl(NO)(NH_3)$_4$]$^{2+}$ (NIMAG = 0)			
Atom	X	Y	Z
Ru	0.332343	–0.019958	0.009070
Cl	0.228936	–2.401114	–0.050771
N	1.815543	–0.276825	1.496112
N	–1.151663	–0.063083	–1.496988
N	1.827170	–0.197866	–1.475959
N	–1.163880	–0.143948	1.497615
H	1.431250	–0.204089	2.435660
H	2.204313	–1.212796	1.393578
H	2.574432	0.398051	1.425419
H	–1.341699	–1.043312	–1.701414
H	–0.853878	0.390593	–2.358100
H	–2.023711	0.377489	–1.211983
H	2.710338	0.223345	–1.196323
H	1.982115	–1.193067	–1.631699
H	1.557051	0.222360	–2.362667
H	–0.939861	0.396627	2.330141
H	–1.249830	–1.124780	1.759971
H	–2.072649	0.174299	1.167968
N	0.399312	1.717856	0.057097
O	0.437680	2.884711	0.092576
trans–[RuCl(NO)(NH_3)$_4$]$^{+}$ (NIMAG = 0)			
Atom	X	Y	Z
Ru	0.375767	–0.052637	0.031838
Cl	0.264911	–2.549919	–0.105304
N	1.880018	–0.277171	1.524375
N	–1.131580	0.039112	–1.454380
N	1.875509	–0.191272	–1.468917
N	–1.145020	–0.217723	1.501974
H	1.536037	–0.067113	2.457850
H	2.187620	–1.247547	1.510246
H	2.679461	0.327023	1.351990
H	–1.784994	–0.728076	–1.313246
H	–0.749170	–0.057103	–2.392086
H	–1.642815	0.919468	–1.418399
H	2.798825	0.046696	–1.116330
H	1.888982	–1.162499	–1.774988
H	1.690151	0.405753	–2.270786
H	–0.880666	0.195369	2.392491
H	–1.305579	–1.214285	1.638349
H	–2.018649	0.214247	1.211369
N	0.411322	1.763341	0.109575
O	–0.226818	2.758828	–0.236321
trans–[RuCl(NO)(NH_3)$_4$]$^{+}$ + 9H_2O (NIMAG = 0)			
Atom	X	Y	Z
Ru	–0.953660	–0.285526	0.193387
N	–0.832449	–2.329586	0.754690
H	0.156633	–2.598820	0.918478
H	–1.375160	–2.531859	1.589350
H	–1.211385	–2.885857	–0.019547
Cl	–3.391796	–0.777354	–0.416574
N	–1.594863	0.304371	2.128268
H	–0.836456	0.777410	2.616664
H	–2.389758	0.950158	2.025261
H	–1.889827	–0.485104	2.696450
N	–1.378133	1.683703	–0.471336
H	–0.546514	2.288313	–0.373607
H	–1.663773	1.672381	–1.446538
H	–2.157427	2.053412	0.082057

N	–0.385565	–0.887112	–1.766943
H	0.641782	–0.947321	–1.817202
H	–0.808976	–1.799302	–1.966854
H	–0.697336	–0.226459	–2.473429
O	1.854436	1.806433	–2.437849
H	1.597259	2.280446	–1.609703
H	2.126235	0.875622	–2.247401
N	0.728276	0.088785	0.668734
O	1.406964	0.696735	1.530893
O	6.057533	–1.300982	0.822150
H	6.470391	–1.855487	1.500113
H	6.723695	–0.901013	0.244374
O	2.524798	–0.803203	–1.885460
H	2.954965	–0.907205	–0.983178
H	2.996141	–1.315030	–2.560265
O	3.524969	–0.991925	0.551215
H	4.522062	–1.099105	0.667996
H	3.169261	–0.241399	1.064165
O	1.858920	–3.002412	1.090506
H	2.552020	–2.307955	0.908143
H	2.209407	–3.719092	1.639305
O	1.078818	3.107260	–0.136308
H	1.487128	2.720703	0.656951
H	1.145946	4.109077	–0.140044
O	–3.769386	1.887411	1.189864
H	–4.417290	2.531022	1.514101
H	–4.194013	1.167301	0.681414
O	1.242931	5.694774	–0.192964
H	0.562259	6.301700	0.133093
H	1.960881	6.179527	–0.626146
O	–2.047267	–3.277458	–1.722196
H	–2.223347	–4.097844	–2.207233
H	–2.865839	–2.764249	–1.566724

$[RuCl(NO)(H_2O)(NH_3)_4]^{+‡} + 8H_2O$ (NIMAG = 1)

Atom	X	Y	Z
Ru	–0.776099	–0.498285	0.026080
N	0.589844	–1.687946	1.157895
H	1.515339	–1.247355	1.275186
H	0.204920	–1.849493	2.084224
H	0.716817	–2.589045	0.690133
Cl	–2.020255	–2.613509	–0.274084
N	–2.244129	–0.208150	1.552478
H	–2.138889	0.719150	1.966367
H	–3.180470	–0.327304	1.153220
H	–2.116590	–0.900625	2.285714
N	–2.261070	0.493536	–1.146342
H	–2.250693	1.477724	–0.863546
H	–2.010433	0.444672	–2.128338
H	–3.189739	0.091330	–0.993875
N	0.483477	–1.138582	–1.567779
H	1.360134	–0.612322	–1.527092
H	0.671417	–2.143260	–1.489537
H	0.039632	–0.939851	–2.459085
O	0.159624	1.400701	–1.075637
H	–0.279854	2.240258	–0.762843
H	1.154049	1.410461	–1.101788
N	0.188084	0.883430	1.521031
O	–0.494342	1.810539	2.091668
O	6.920940	0.443681	–0.416054
H	7.498683	–0.175328	0.053358
H	7.327357	0.747789	–1.240492
O	2.711743	0.952854	–1.443699

H	3.445322	1.020225	–0.761722
H	3.041848	1.170233	–2.328551
O	4.590361	1.092968	0.387800
H	5.525223	0.853643	0.072918
H	4.593359	1.919508	0.894340
O	3.325691	–0.952570	1.563769
H	3.835052	–0.188220	1.181715
H	3.771582	–1.310126	2.346188
O	–1.416296	3.186985	–0.066124
H	–1.231656	2.986991	0.877569
H	–1.704406	4.127926	–0.230077
O	–4.599892	–0.867976	–0.061641
H	–5.567428	–0.813460	–0.040849
H	–4.292622	–1.782807	–0.209539
O	–2.176015	5.645012	–0.527427
H	–3.098684	5.938887	–0.552590
H	–1.574322	6.382482	–0.707728
O	0.740028	–3.940313	–0.806390
H	1.256112	–4.738180	–0.998186
H	–0.216548	–4.130750	–0.764292

trans–$[RuCl(H_2O)(NH_3)_4]^+ + NO + 8H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.878336	–0.516514	–0.320764
N	0.111065	–0.459610	1.525947
H	1.066402	–0.065754	1.422965
H	–0.390572	0.120821	2.205232
H	0.203942	–1.420159	1.871294
Cl	–2.426942	–2.214420	0.528391
N	–2.203363	1.026941	0.278147
H	–1.912045	1.907944	–0.144776
H	–3.150950	0.789566	–0.028411
H	–2.179230	1.162291	1.292438
N	–1.900366	–0.564592	–2.180881
H	–1.554239	0.213532	–2.737413
H	–1.758469	–1.424531	–2.702473
H	–2.905644	–0.440537	–1.998560
N	0.471773	–2.042305	–0.924177
H	1.323812	–1.617073	–1.301215
H	0.687381	–2.615493	–0.101334
H	0.069026	–2.648217	–1.633499
O	0.340237	0.875273	–1.058425
H	0.279349	1.848949	–0.658770
H	1.219868	0.579334	–1.463809
N	–1.147801	1.921574	3.020494
O	–0.365456	2.874025	2.582811
O	5.909227	–1.929627	–0.038851
H	6.150221	–2.254922	0.840560
H	6.183392	–2.548670	–0.730809
O	2.497832	–0.109256	–1.994015
H	3.342846	–0.000526	–1.451251
H	2.678467	–0.142247	–2.944624
O	4.552996	0.182280	–0.446094
H	5.113812	–0.651284	–0.288954
H	5.113368	0.953964	–0.620513
O	2.747421	0.539647	1.522263
H	3.454279	0.445281	0.830336
H	3.001061	1.188682	2.195135
O	0.034307	3.073936	–0.014354
H	–0.075842	3.071340	0.980245
H	0.173021	3.977006	–0.414966
O	–4.488087	–0.318721	–0.977929
H	–5.400532	–0.117277	–1.236377

H	–4.443712	–1.120653	–0.423658
O	0.393576	5.416826	–1.089385
H	–0.321985	5.995006	–1.392441
H	1.252406	5.856481	–1.174643
O	0.292034	–3.382647	1.657707
H	0.719135	–4.070468	2.191074
H	–0.665640	–3.548598	1.563678

trans–$[RuCl(HNO)(NH_3)_4]^{2+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–2.439508	–0.505319	4.091912
N	–3.213058	–1.993792	2.802377
N	–1.683864	0.558680	2.675006
N	–4.216757	0.603687	3.838869
N	–1.723123	0.950353	5.441903
N	–0.674758	–1.634605	4.391702
Cl	–3.446207	–1.621116	5.924122
H	–2.386396	1.064194	6.206541
H	–0.829253	0.696165	5.856986
H	–1.612973	1.853012	4.978903
H	–0.797987	–2.148367	5.263753
H	–0.503497	–2.319753	3.657397
H	0.165961	–1.065825	4.473653
H	–3.883268	–2.538286	3.344392
H	–3.690374	–1.620771	1.984353
H	–2.500125	–2.638029	2.464365
H	–4.707541	0.679216	4.728434
H	–4.008890	1.545518	3.505921
H	–4.857645	0.171946	3.176798
O	–1.790510	1.806756	2.548067
H	–1.119669	0.119802	1.925196

trans–$[RuCl(HNO)(NH_3)_4]^{2+}$ + $9H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.917941	–0.660372	0.131042
N	0.527189	–2.206043	0.166456
H	1.315484	–1.972929	0.783972
H	0.120872	–3.091034	0.461499
H	0.859660	–2.326154	–0.804336
Cl	–2.050326	–1.774454	–1.784318
N	–2.215491	–1.748494	1.384218
H	–1.732800	–2.333493	2.062194
H	–2.810710	–1.078266	1.905535
H	–2.801604	–2.337230	0.796098
N	–2.356630	0.849173	0.026849
H	–1.959609	1.794436	–0.130075
H	–2.996599	0.633099	–0.735039
H	–2.886516	0.862186	0.912486
N	0.300322	0.301470	–1.279247
H	1.106719	0.816165	–0.887621
H	0.659336	–0.443808	–1.896573
H	–0.238045	0.948041	–1.868032
O	1.039896	3.686821	0.600495
H	0.161532	3.612187	0.156681
H	1.657136	3.001860	0.247439
N	–0.068123	0.126195	1.643217
O	–0.592585	0.911188	2.480236
H	0.934419	–0.171792	1.889014
O	5.956641	–1.000590	–0.217185
H	6.219307	–1.894511	0.045321
H	6.414302	–0.719867	–1.022730
O	2.652591	1.744278	–0.491754
H	3.313878	1.272263	0.095697
H	3.085352	2.064476	–1.298907

O	4.324346	0.432319	1.087203
H	4.998834	–0.132629	0.570754
H	4.770311	1.006523	1.729213
O	2.335191	–0.921430	2.057310
H	3.149732	–0.427160	1.719090
H	2.518455	–1.380363	2.891193
O	–1.366935	3.405286	–0.722561
H	–1.985087	4.144869	–0.617477
H	–1.212694	3.188769	–1.686640
O	–3.597519	0.402024	2.572302
H	–3.104432	0.855726	3.275380
H	–4.550791	0.428536	2.751074
O	–0.875906	2.419176	–3.094229
H	–1.621380	2.155004	–3.657277
H	–0.143223	2.744869	–3.641534
O	0.983199	–2.134806	–2.630522
H	1.706446	–2.408731	–3.215024
H	0.114416	–2.399194	–2.984636

$[RuCl(HNO)(H_2O)(NH_3)_4]^{2+‡} + 8H_2O$ (NIMAG = 1)

Atom	X	Y	Z
Ru	–0.695360	–0.572588	0.101020
N	0.830979	–1.819705	0.943708
H	1.641504	–1.261624	1.234661
H	0.483412	–2.326473	1.753287
H	1.122667	–2.500402	0.232759
Cl	–1.659767	–2.608623	–0.797174
N	–2.176803	–0.796115	1.626860
H	–2.197002	0.025238	2.229419
H	–3.093303	–0.932783	1.184643
H	–1.971931	–1.608852	2.201589
N	–2.249827	0.513174	–0.867526
H	–2.303290	1.465627	–0.492565
H	–2.074164	0.582166	–1.866327
H	–3.144204	0.030149	–0.726806
N	0.595291	–0.607973	–1.596122
H	1.335604	0.097629	–1.532199
H	1.008141	–1.543929	–1.680733
H	0.060783	–0.423411	–2.441338
O	0.159306	1.578882	0.049699
H	–0.513951	2.331105	0.088828
H	1.019077	1.769979	–0.441876
N	0.111305	0.561620	1.996610
O	–0.527211	1.191810	2.862822
H	1.158268	0.727101	2.008211
O	6.074778	–0.355156	–0.776275
H	6.495569	–1.074945	–0.284419
H	6.333575	–0.366073	–1.708992
O	2.365661	1.753046	–1.240790
H	3.222622	1.635980	–0.724247
H	2.484750	2.308696	–2.024516
O	4.460514	1.317543	0.235365
H	5.127141	0.658843	–0.165807
H	4.910358	2.106910	0.574449
O	2.801958	0.196499	1.961673
H	3.467845	0.617306	1.341758
H	3.215382	–0.029784	2.809168
O	–1.765822	3.265242	0.144743
H	–2.091906	3.544717	1.012886
H	–1.918194	3.977640	–0.554656
O	–4.447873	–1.220697	–0.107676
H	–5.412343	–1.145900	–0.042640
H	–4.184088	–2.059044	–0.526999

O	–2.134618	5.045219	–1.663347
H	–2.925845	5.106755	–2.218067
H	–1.499458	5.742650	–1.881735
O	1.353716	–3.407107	–1.424117
H	2.071921	–3.976223	–1.740821
H	0.483048	–3.817864	–1.571325

trans–$[RuCl(H_2O)(NH_3)_4]^{2+}$ + HNO + $8H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.861827	–0.555552	–0.070128
N	0.679026	–1.559598	0.975010
H	1.440720	–0.922404	1.254367
H	0.307732	–1.987180	1.820319
H	1.037961	–2.317413	0.387235
Cl	–2.177132	–2.595356	0.005239
N	–1.753887	0.072932	1.742112
H	–1.229052	0.874558	2.110282
H	–2.738603	0.300270	1.587522
H	–1.722344	–0.670230	2.436322
N	–2.433061	0.452605	–1.077204
H	–2.251196	1.460577	–1.046513
H	–2.532735	0.166062	–2.046891
H	–3.310174	0.252114	–0.578185
N	0.105163	–1.180438	–1.852102
H	0.943427	–0.608092	–1.985623
H	0.382188	–2.164270	–1.735860
H	–0.480301	–1.098234	–2.678588
O	0.198211	1.151306	–0.167717
H	–0.335675	2.022323	–0.243108
H	1.069547	1.142909	–0.704295
N	0.536099	1.935725	2.542028
O	0.859098	3.119803	2.769658
H	1.391477	1.357514	2.283410
O	5.698247	–1.515654	–0.576955
H	6.013774	–2.125252	0.105639
H	5.904696	–1.841820	–1.464710
O	2.288064	0.934956	–1.561099
H	3.155851	0.811709	–1.059580
H	2.406346	1.464427	–2.363316
O	4.402604	0.608976	–0.094609
H	4.943739	–0.232693	–0.291021
H	4.978075	1.386934	–0.029276
O	2.756400	0.234177	1.949939
H	3.425615	0.408849	1.225230
H	3.195228	–0.103065	2.746693
O	–1.286581	3.161896	–0.471159
H	–1.685298	3.615986	0.285321
H	–1.128567	3.792944	–1.247113
O	–4.452864	–0.396941	0.736565
H	–5.388540	–0.210075	0.908385
H	–4.285151	–1.357260	0.699912
O	–0.864964	4.712574	–2.453698
H	–1.476186	4.835563	–3.194460
H	–0.070384	5.255302	–2.560871
O	0.663296	–3.805449	–0.897690
H	1.183085	–4.577031	–1.170242
H	–0.239104	–4.061417	–0.629191

trans–$[RuCl(H_2O)(NH_3)_4]^{2+}$ + HNO + $8H_2O$ (Cl^- → HNO substitution) (NIMAG = 0)

Atom	X	Y	Z
Ru	0.468745	–0.127487	–0.740075
N	–1.431231	–0.974707	–1.132932
O	1.206969	–1.189985	–2.386415
N	–0.045705	1.472915	–2.005461

N	2.372199	0.720865	–0.373836
N	1.031106	–1.746322	0.498476
Cl	–0.434825	0.996112	1.171905
N	–3.651081	1.037863	0.887905
H	–3.377310	0.046737	1.174353
O	–4.222770	1.654279	1.805794
H	1.505436	–2.155324	–2.244222
H	1.716277	–0.750990	–3.082750
H	1.710796	–1.394554	1.195352
H	0.225392	–2.132064	0.983323
H	1.454514	–2.495135	–0.054448
H	2.644593	0.501053	0.593875
H	3.073290	0.330141	–0.998988
H	2.328469	1.737994	–0.524211
H	0.532477	2.296355	–1.776159
H	0.102020	1.229774	–2.982954
H	–1.051617	1.678697	–1.882231
H	–1.885235	–1.302050	–0.269220
H	–2.028794	–0.254199	–1.550995
H	–1.340644	–1.750456	–1.784140
O	2.839368	–0.426057	2.227583
H	2.413880	0.023303	2.973754
H	3.746171	–0.773240	2.483948
O	0.562787	4.061126	1.225051
H	0.132588	3.216134	1.464662
H	0.032154	4.822761	1.501033
O	–4.683592	–3.435037	1.073586
H	–4.563007	–4.259834	0.580656
H	–5.587269	–3.362289	1.414214
O	–2.876739	–1.611461	1.359076
H	–3.574006	–2.332359	1.262592
H	–2.364360	–1.733605	2.173256
O	1.732690	3.472451	–0.997950
H	1.323054	3.862069	–0.166181
H	2.282910	4.112827	–1.471795
O	–2.841397	1.566848	–1.651997
H	–3.230575	1.528906	–0.728896
H	–3.483051	1.891484	–2.301172
O	5.189533	–1.335721	2.843061
H	5.362671	–2.220114	3.197964
H	6.009692	–0.826250	2.766711
O	1.912491	–3.546430	–1.819572
H	2.844522	–3.811811	–1.858949
H	1.330499	–4.302821	–1.992283
Ru	0.468745	–0.127487	–0.740075
N	–1.431231	–0.974707	–1.132932

trans–[RuCl(H_2O)(NH_3)$_4$]$^{2+‡}$ + HNO···H_2O + 7H_2O (NIMAG = 1)

Atom	X	Y	Z
Ru	0.205083	–0.324104	–0.454447
N	–1.368654	–1.752485	–0.195335
O	0.924370	–1.741130	–1.767022
N	–0.458889	0.644883	–2.232621
N	1.933923	0.828738	–0.806772
N	1.183980	–1.406202	1.091443
Cl	–0.000879	1.260946	1.503348
N	–2.138606	0.753658	–0.152117
H	–2.505375	0.445581	0.805533
O	–2.520026	1.874176	–0.558975
H	1.289019	–2.631343	–1.433292
H	0.931817	–1.653142	–2.729230
H	2.014824	–0.860730	1.377857
H	0.565775	–1.493545	1.892703

H	1.467285	–2.338050	0.786612
H	2.504185	0.855792	0.050061
H	2.483730	0.406856	–1.551789
H	1.642965	1.774162	–1.097194
H	–0.436889	1.660737	–2.091434
H	0.158964	0.447593	–3.016118
H	–1.395171	0.296705	–2.455613
H	–1.892825	–1.577839	0.668336
H	–1.985404	–1.637317	–1.008355
H	–1.006260	–2.700768	–0.182947
O	3.339707	0.366720	1.655581
H	3.098345	0.985087	2.362171
H	4.314792	0.132865	1.691360
O	–0.235646	4.231905	0.481054
H	–0.302708	3.400376	1.000014
H	–1.006662	4.800989	0.622808
O	–5.141968	–1.327365	2.857723
H	–5.387156	–2.252083	3.007858
H	–5.898561	–0.739509	2.998685
O	–2.800069	–0.548666	2.105427
H	–3.709635	–0.847781	2.415963
H	–2.220711	–0.320837	2.848665
O	0.658556	3.247568	–1.738940
H	0.303226	3.764494	–0.952946
H	0.990768	3.832730	–2.435647
O	–2.842493	–1.052497	–2.647408
H	–3.748212	–0.714718	–2.553340
H	–2.789819	–1.631977	–3.425195
O	5.858338	–0.268700	1.706612
H	6.229045	–1.001502	2.220073
H	6.551065	0.191677	1.210322
O	1.830718	–3.849570	–0.730621
H	2.781136	–4.040812	–0.756859
H	1.315573	–4.668905	–0.669943

trans–$[Ru(HNO)(H_2O)(NH_3)_4]^{3+}$ + Cl^- + $8H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.861632	–0.129804	–0.529858
N	–2.786671	–0.078358	0.334470
O	–1.668297	–1.513231	–1.915689
N	–1.339591	1.532529	–1.724665
N	0.911656	–0.259375	–1.605073
N	–0.221599	–1.760497	0.634032
Cl	3.852157	0.981713	1.507421
N	–0.202570	1.027301	0.823010
H	–0.103423	0.618636	1.802724
O	0.039235	2.260664	0.746341
H	–1.683641	–2.502470	–1.688968
H	–2.010074	–1.312318	–2.796959
H	0.815729	–1.824900	0.532339
H	–0.402207	–1.588102	1.629578
H	–0.651372	–2.635821	0.330337
H	1.653151	–0.712697	–1.029235
H	0.737116	–0.828989	–2.430254
H	1.212150	0.690882	–1.900944
H	–0.456408	2.051900	–1.893681
H	–1.749345	1.284309	–2.621712
H	–2.004911	2.134629	–1.218718
H	–2.821937	–0.318970	1.333249
H	–3.166985	0.879091	0.234018
H	–3.375749	–0.727258	–0.182884
O	2.529665	–1.534880	0.227691
H	3.004088	–0.816581	0.715247

H	3.125459	–2.314994	0.032752
O	2.984520	3.200987	–0.459699
H	3.282573	2.510348	0.190016
H	2.970948	4.079331	–0.052536
O	–3.019953	–0.449207	3.302688
H	–3.426291	–1.287226	3.577835
H	–3.538846	0.299156	3.640046
O	–0.429228	–0.319138	3.121921
H	–1.394891	–0.349886	3.381733
H	0.167379	–0.397649	3.880222
O	1.300048	2.429028	–2.222527
H	1.947060	2.797009	–1.526697
H	1.536562	2.725132	–3.114339
O	–3.423929	2.667589	–0.092260
H	–3.216106	3.291424	0.622382
H	–4.241147	2.939452	–0.540810
O	4.046227	–3.589300	–0.300052
H	4.177702	–4.341681	0.295743
H	4.616239	–3.663339	–1.079743
O	–1.580636	–3.901778	–1.089369
H	–0.951759	–4.542782	–1.456315
H	–2.375754	–4.350444	–0.761592

trans–[Ru(HNO)(H_2O)(NH_3)$_4$]$^{3+}$ + 9H_2O (NIMAG = 0)

Atom	X	Y	Z
Ru	0.306810	–0.535841	–0.709842
N	0.021775	–2.692749	–0.741638
O	2.441250	–0.825775	–0.422568
N	0.693282	–0.317867	–2.783643
N	0.366466	1.499316	–0.415756
N	0.161321	–0.606997	1.389694
O	–1.766593	2.007076	1.029985
N	–1.553784	–0.356714	–1.102583
H	–2.205352	2.911220	1.091057
H	–2.233398	–1.115727	–0.784357
H	–2.199738	1.338647	1.598795
O	–2.073007	0.544137	–1.793491
H	3.154777	–0.226001	0.036520
H	2.864772	–1.653035	–0.698655
H	–0.784157	–0.465344	1.786917
H	0.533972	–1.481468	1.755252
H	0.793336	0.152455	1.730200
H	–0.524469	1.755332	0.141745
H	1.159120	1.780619	0.169860
H	0.345998	2.007565	–1.308990
H	0.133808	–0.912793	–3.394525
H	0.468961	0.672236	–3.041327
H	1.677671	–0.483447	–2.990994
H	–0.943841	–2.886930	–0.430569
H	0.125219	–3.096439	–1.673423
H	0.665354	–3.190584	–0.128096
O	–2.422222	–0.228731	2.602013
H	–3.165770	–0.860824	2.444519
H	–2.408067	0.047927	3.533789
O	–2.904960	4.325762	1.206095
H	–3.688720	4.596679	0.704273
H	–2.642002	5.020076	1.829391
O	–2.909054	–2.544570	–0.257316
H	–3.430502	–2.468385	0.591575
H	–3.401223	–3.093038	–0.892451
O	–4.340502	–2.145928	1.995668
H	–5.234785	–1.793960	1.833042
H	–4.394651	–2.873439	2.641786

O	0.068852	2.356247	–3.241472
H	0.621823	2.969539	–3.755553
H	–0.871307	2.561332	–3.385313
O	4.234276	0.547041	0.734155
H	4.956180	0.043032	1.287754
H	4.660213	1.257870	0.226151
O	2.011217	1.418805	1.939885
H	1.943800	2.079334	2.647048
H	2.951971	1.194920	1.721100
O	6.014144	–0.617709	2.063268
H	6.732147	–1.141167	1.674759
H	6.188596	–0.434963	2.999510

$[Ru(HNO)(H_2O)_2(NH_3)_4]^{3+‡}$ + $8H_2O$ (NIMAG = 1)

Atom	X	Y	Z
Ru	–0.423849	–0.262641	–0.409071
N	0.622964	0.607651	–2.071607
O	–1.986060	0.889983	–1.051015
N	–1.378362	–1.845689	–1.484787
N	–1.679186	–0.839905	1.196507
N	0.290863	1.436767	0.664072
O	1.110097	–1.183642	1.066679
N	1.313881	–1.741241	–1.035215
H	0.807871	–1.952454	1.631692
H	2.292133	–1.340947	–0.997719
H	1.821715	–0.603311	1.488262
O	1.259967	–2.966937	–1.241209
H	–2.169007	1.850961	–0.708639
H	–2.798689	0.458456	–1.352467
H	1.217337	1.260713	1.062935
H	0.341871	2.292974	0.110556
H	–0.364403	1.608838	1.437897
H	–1.216400	–1.512383	1.808586
H	–1.909393	0.012790	1.724986
H	–2.546958	–1.263915	0.852180
H	–0.810753	–2.690152	–1.411087
H	–2.314329	–2.045761	–1.107516
H	–1.468484	–1.623058	–2.473915
H	1.633161	0.647847	–1.890020
H	0.477306	0.072726	–2.924256
H	0.261070	1.543327	–2.232873
O	2.795760	0.508739	1.984414
H	3.653265	0.682464	1.508144
H	2.861309	0.706656	2.930051
O	0.033647	–3.053249	2.508482
H	–0.142424	–3.938976	2.154023
H	0.147111	–3.089520	3.471083
O	3.435470	–0.083183	–1.489581
H	4.028630	0.313388	–0.799534
H	3.932040	–0.254559	–2.305281
O	4.953922	0.927222	0.501988
H	5.733584	0.384538	0.706420
H	5.213503	1.857923	0.400106
O	–3.913694	–2.212890	–0.134751
H	–4.730967	–1.762026	–0.402024
H	–4.122043	–3.103481	0.191285
O	–2.402601	3.177118	–0.109676
H	–1.591028	3.780470	–0.221111
H	–3.228164	3.623753	–0.351686
O	–2.097518	1.838360	2.225271
H	–2.320275	2.151979	3.114097
H	–2.411309	2.460213	1.523293
O	–0.200497	4.411560	–0.373364

H	0.108533	4.703299	–1.245144
H	0.164499	4.975712	0.326083

trans–$[Ru(H_2O)_2(NH_3)_4]^{3+}$ + HNO + $8H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.114406	–0.443786	0.064864
N	0.783530	0.445573	–1.652779
O	–1.815142	–0.840930	–1.029589
N	0.676666	–2.376838	–0.436777
N	–1.059984	–1.258939	1.765910
N	–0.847040	1.448182	0.682548
O	1.547708	–0.057416	1.102018
N	3.876834	–0.640311	–2.687109
H	2.369855	–0.641999	0.988223
H	4.389543	–0.521846	–3.596290
H	1.674196	0.810615	1.630304
O	4.630137	–1.115772	–1.819128
H	–2.796157	–0.500582	–0.912567
H	–1.790992	–1.548890	–1.691010
H	–0.275623	1.786600	1.460699
H	–0.765356	2.152325	–0.053358
H	–1.817726	1.356476	1.012972
H	–0.483439	–1.091542	2.588860
H	–1.964418	–0.776337	1.895990
H	–1.199424	–2.273536	1.679729
H	1.646142	–2.422669	–0.104269
H	0.141660	–3.114351	0.046388
H	0.690622	–2.592360	–1.432049
H	0.930518	1.455251	–1.461488
H	1.676401	0.029612	–1.926148
H	0.150927	0.375575	–2.448997
O	1.683089	2.142366	2.336328
H	1.997078	2.978340	1.894184
H	1.816227	2.178068	3.296662
O	3.451153	–1.679853	0.623681
H	4.021183	–1.511328	–0.162029
H	3.934607	–2.171545	1.307303
O	0.832237	3.225500	–1.058839
H	1.407928	3.678475	–0.396935
H	0.628549	3.829090	–1.792221
O	2.373393	4.368663	0.990184
H	3.317375	4.509587	0.795605
H	1.990097	5.195682	1.334692
O	–0.921425	–4.183167	1.249696
H	–1.660204	–4.720108	0.914274
H	–0.444195	–4.701777	1.921306
O	–4.236154	–0.185677	–0.761980
H	–4.690664	0.567493	–1.314890
H	–4.829422	–0.955586	–0.728301
O	–3.340408	0.478291	1.700919
H	–3.856685	0.778192	2.466098
H	–3.910008	0.302042	0.911829
O	–5.420613	1.590931	–2.079444
H	–5.544774	1.569237	–3.040891
H	–6.001818	2.251204	–1.671012

trans–$[Ru(H_2O)_2(NH_3)_4]^{3+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	0.000012	0.000006	–0.000015
N	–1.528688	1.508439	0.001989
O	–0.001201	0.001894	–2.051472
N	1.532359	1.504754	0.000467
N	1.528679	–1.508535	–0.002035
N	–1.532299	–1.504876	–0.000389

O	0.001100	–0.001680	2.051497
H	0.002453	0.796376	2.613555
H	0.000313	–0.800429	2.612625
H	–0.002681	–0.795931	–2.613913
H	–0.000358	0.800862	–2.612286
H	–1.191654	–2.469016	–0.001616
H	–2.145118	–1.425061	0.816674
H	–2.146400	–1.423483	–0.816337
H	2.142963	–1.429493	0.814008
H	1.186123	–2.472003	–0.002140
H	2.141613	–1.428833	–0.819026
H	2.146119	1.423268	0.816660
H	2.145457	1.424587	–0.816357
H	1.192033	2.469010	0.001370
H	–2.141884	1.428205	0.818730
H	–1.186452	2.472025	0.002604
H	–2.142619	1.429479	–0.814319

trans–$[Ru(H_2O)_2(NH_3)_4]^{2+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	0.000009	0.000009	0.000008
N	–0.069341	1.925708	0.965709
O	–2.146091	0.006278	–0.004050
N	0.079744	0.965639	–1.925296
N	–0.077129	–1.925225	–0.966004
N	0.066686	–0.966082	1.925589
O	2.146097	–0.006355	0.004016
H	2.697400	–0.719806	–0.352092
H	2.700311	0.703765	0.362256
H	–2.701207	–0.349053	0.706824
H	–2.696495	0.364888	–0.716941
H	1.047425	–1.095041	2.176619
H	–0.364662	–0.427015	2.676361
H	–0.369214	–1.888018	1.943496
H	0.351250	–2.678090	–0.427491
H	–1.059230	–2.171517	–1.093751
H	0.357542	–1.945251	–1.888479
H	1.062178	1.088875	–2.172547
H	–0.351837	0.429071	–2.677721
H	–0.350712	1.890101	–1.944913
H	0.361726	1.943159	1.889931
H	0.365777	2.675900	0.428861
H	–1.050425	2.177982	1.089502

HNO (NIMAG = 0)

Atom	X	Y	Z
H	–2.941935	–0.511927	1.133820
N	–2.124484	–1.089585	0.795407
O	–2.513865	–2.229771	0.494340

HNO^+ (NIMAG = 0)

Atom	X	Y	Z
N	–2.227554	–1.158818	0.791676
H	–2.911388	–0.429618	1.155107
O	–2.441342	–2.242847	0.476784

H_2O (NIMAG = 0)

Atom	X	Y	Z
O	2.165606	–0.002100	0.017104
H	2.684513	0.242812	–0.766432
H	2.676920	0.204209	0.816579

H_3O^+ (NIMAG = 0)

Atom	X	Y	Z
O	–2.438338	–2.283036	0.419278
H	–2.348430	–1.746182	1.221378
H	–2.671335	–3.221378	0.488032
H	–2.334033	–1.872394	–0.452590

NO (NIMAG = 0)

Atom	X	Y	Z
N	0.000000	0.000000	0.110015
O	0.000000	0.000000	1.289985

trans–[Ru(NO)(NH$_3$)$_4$(P(OEt)$_3$)]$^{3+}$ (NIMAG = 0)			
Atom	X	Y	Z
Ru	1.607374	–0.085500	–0.060464
N	1.424911	–1.497199	1.514103
H	2.121524	–1.339586	2.240289
H	0.497042	–1.409032	1.939272
H	1.538630	–2.457038	1.195970
P	–0.863968	–0.102005	–0.079854
N	1.245564	1.470487	1.344433
H	2.110334	1.943837	1.599171
H	0.611946	2.174368	0.963906
H	0.824218	1.114718	2.201583
N	1.465325	1.371560	–1.592553
H	2.164248	2.101912	–1.470318
H	1.593423	0.982093	–2.524168
H	0.539290	1.807199	–1.553395
N	1.654639	–1.624249	–1.525566
H	2.571875	–1.670847	–1.965742
H	1.466096	–2.542378	–1.127401
H	0.976579	–1.475754	–2.271196
N	3.357921	–0.000221	0.065691
O	4.509945	0.052309	0.174978
O	–1.940267	–0.967779	–1.012775
C	–2.356799	–2.379388	–0.799003
H	–2.405482	–2.575560	0.272593
H	–1.598828	–3.017546	–1.250515
C	–3.698720	–2.539118	–1.462260
H	–3.637208	–2.310288	–2.526124
H	–4.444908	–1.892917	–0.999974
H	–4.024843	–3.575790	–1.353172
O	–1.241630	–0.390088	1.519078
C	–2.566666	–0.282423	2.189386
H	–2.743313	–1.267760	2.615929
H	–3.331031	–0.079354	1.437446
C	–2.498832	0.789357	3.245235
H	–2.313905	1.771896	2.809928
H	–1.716026	0.569540	3.971369
H	–3.453915	0.825062	3.774018
O	–1.229050	1.453134	–0.545131
C	–2.580511	2.013401	–0.821233
H	–2.981692	2.352585	0.133166
H	–3.201333	1.215958	–1.227496
C	–2.404153	3.149213	–1.793310
H	–2.007780	2.795278	–2.745356
H	–1.738984	3.912517	–1.388626
H	–3.377315	3.609457	–1.977781

trans–[Ru(NO)(NH$_3$)$_4$(P(OEt)$_3$)]$^{2+}$ (NIMAG = 0)			
Atom	X	Y	Z
Ru	1.573308	–0.151519	–0.089094
N	1.438672	–1.321672	1.691522
H	2.213236	–1.115054	2.317246
H	0.566350	–1.091181	2.170739
H	1.446794	–2.322638	1.513977
P	–0.839436	–0.106038	–0.067988
N	1.416901	1.582417	1.139898
H	2.325464	1.840271	1.521356
H	1.059883	2.384442	0.624165
H	0.780267	1.416962	1.918458
N	1.461477	1.093526	–1.815577
H	2.157426	1.834446	–1.777956
H	1.612766	0.575339	–2.677196
H	0.532706	1.520099	–1.854203

N	1.795758	–1.881265	–1.327501
H	2.754205	–1.903586	–1.669775
H	1.631048	–2.748821	–0.822531
H	1.173287	–1.878487	–2.132165
N	3.427673	–0.027958	0.003525
O	4.337480	0.617974	0.478659
O	–2.057341	–1.096110	–0.709270
C	–2.226129	–2.511396	–0.332732
H	–2.238733	–2.592597	0.756170
H	–1.381139	–3.079423	–0.723697
C	–3.527147	–2.978056	–0.934769
H	–3.509592	–2.879095	–2.020500
H	–4.367005	–2.405496	–0.540032
H	–3.681237	–4.030749	–0.688255
O	–1.219317	–0.011055	1.577813
C	–2.564229	0.133579	2.169865
H	–2.660087	–0.694091	2.871480
H	–3.315841	0.012550	1.386865
C	–2.672117	1.467657	2.867537
H	–2.570852	2.297505	2.166516
H	–1.903994	1.564228	3.635626
H	–3.649495	1.545077	3.349077
O	–1.270661	1.324473	–0.835217
C	–2.640114	1.778405	–1.150951
H	–3.096059	2.134566	–0.226041
H	–3.205572	0.929188	–1.531860
C	–2.521108	2.884926	–2.167860
H	–2.062466	2.521533	–3.088272
H	–1.927042	3.712201	–1.778020
H	–3.517937	3.261936	–2.406726

trans–$[Ru(NO)(NH_3)_4(P(OEt)_3)]^{2+}$ + $9H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–1.142303	–0.674706	0.378488
N	–0.753944	–0.764337	2.485441
H	–1.254868	–1.542125	2.906845
H	0.235621	–0.888731	2.688393
H	–1.075860	0.111219	2.924896
P	1.154795	0.072087	0.079658
N	–0.543439	–2.713082	0.146562
H	–1.380510	–3.294050	0.147219
H	–0.024301	–2.918572	–0.715721
H	0.068354	–3.041348	0.896205
N	–1.331518	–0.469214	–1.724813
H	–2.256518	–0.802426	–2.016320
H	–1.247544	0.531548	–1.977210
H	–0.609028	–0.986910	–2.218154
N	–1.896825	1.307511	0.523206
H	–2.894377	1.258745	0.232962
H	–1.824015	1.675705	1.473599
H	–1.440984	1.922578	–0.155782
O	–4.415224	1.132626	–0.662351
H	–4.433937	0.348205	–1.256691
H	–5.325131	1.435137	–0.407886
N	–2.854126	–1.323208	0.598491
O	–3.523913	–2.342094	0.508937
O	1.684550	1.710299	0.106304
C	1.462084	2.597486	1.270608
H	1.527771	2.008262	2.186518
H	0.457634	3.011718	1.186206
C	2.512126	3.680187	1.240147
H	2.443664	4.266071	0.322883
H	3.513777	3.257047	1.317272

H	2.355621	4.353321	2.085590
O	2.264327	–0.637715	1.180285
C	3.557986	–0.009991	1.582181
H	3.349495	0.583507	2.471799
H	3.906427	0.643144	0.782501
C	4.556779	–1.100812	1.878090
H	4.750399	–1.718156	0.999756
H	4.230753	–1.736979	2.702213
H	5.499251	–0.633935	2.173484
O	1.683050	–0.316829	–1.455170
C	3.097293	–0.351221	–1.889753
H	3.549445	–1.240063	–1.445720
H	3.614323	0.536523	–1.522551
C	3.099898	–0.426426	–3.395245
H	2.633403	0.457707	–3.831137
H	2.569097	–1.313022	–3.744416
H	4.131376	–0.481669	–3.750376
O	–1.044396	2.326361	–2.122027
H	–1.733758	2.879102	–2.519122
H	–0.124878	2.700790	–2.283366
O	–4.175233	–1.102349	–2.268765
H	–4.497608	–1.930606	–1.875289
H	–4.458871	–1.044310	–3.195688
O	2.148580	–3.349537	1.148037
H	2.308160	–2.382713	1.278316
H	2.536571	–3.883870	1.856066
O	–6.837482	1.969453	0.036308
H	–7.342605	1.633579	0.792025
H	–7.335973	2.658972	–0.427452
O	5.293603	1.843175	–0.650343
H	5.243230	2.808018	–0.749401
H	6.218142	1.561029	–0.745552
O	1.544699	–3.960300	–1.349886
H	1.947353	–3.830283	–0.447928
H	2.208521	–3.883786	–2.051352
O	1.416791	3.091897	–2.173168
H	1.740562	2.587582	–1.387207
H	2.089565	3.182486	–2.862434
O	–1.705091	1.755881	3.475080
H	–2.570690	1.804010	3.912589
H	–1.089760	2.377310	3.896789

$[Ru(H_2O)(NO)(NH_3)_4(P(OEt)_3)]^{2+‡}$ + $8H_2O$ (NIMAG = 1)

Atom	X	Y	Z
Ru	–1.260257	0.094173	–0.051627
N	–1.127982	0.520637	–2.165008
H	–1.888065	1.154530	–2.399273
H	–0.249511	0.962265	–2.423548
H	–1.229235	–0.342755	–2.713013
P	0.970116	–0.066421	–0.047132
N	–0.845439	2.015916	0.885685
H	–1.675722	2.360853	1.360875
H	–0.104056	1.903198	1.575369
H	–0.531724	2.713808	0.200811
N	–1.356597	–0.560409	1.966508
H	–2.256089	–0.318727	2.391384
H	–1.242403	–1.586867	1.987524
H	–0.608756	–0.158609	2.527362
N	–1.645985	–1.893768	–0.616933
H	–2.651684	–1.905544	–0.410612
H	–1.475701	–2.125147	–1.597721
H	–1.191472	–2.559787	0.019766
O	–3.805106	–0.696800	0.393105

H	–4.056261	–0.543025	1.337126
H	–4.524504	–0.395336	–0.226368
N	–2.948877	1.659405	–0.688078
O	–3.449932	2.457212	0.081172
O	1.852459	–1.519608	–0.272461
C	1.827804	–2.276362	–1.545681
H	1.743649	–1.571864	–2.374264
H	0.947578	–2.918481	–1.531563
C	3.101648	–3.078684	–1.635386
H	3.184595	–3.776873	–0.801779
H	3.974057	–2.425436	–1.640593
H	3.094746	–3.655596	–2.562541
O	1.757575	0.968267	–1.168143
C	3.156120	0.799522	–1.653568
H	3.078823	0.359028	–2.647293
H	3.688744	0.113320	–0.995187
C	3.826486	2.150478	–1.703740
H	3.862684	2.616148	–0.717941
H	3.323212	2.826632	–2.395958
H	4.853111	2.016888	–2.052385
O	1.562503	0.340554	1.469294
C	2.983629	0.566086	1.812669
H	3.234689	1.577705	1.488809
H	3.608609	–0.148788	1.276513
C	3.112439	0.419949	3.307755
H	2.848359	–0.589409	3.625242
H	2.471164	1.132420	3.828303
H	4.147075	0.613294	3.599936
O	–0.726302	–3.342387	1.717157
H	–1.206936	–4.129420	2.012527
H	0.267900	–3.431655	1.851033
O	–4.140307	–0.168333	3.004988
H	–4.464177	0.709420	3.262670
H	–4.421689	–0.832404	3.654122
O	0.716128	3.455278	–1.069431
H	1.167953	2.591063	–1.245765
H	0.431427	3.886440	–1.889616
O	–5.758498	–0.010366	–1.254360
H	–5.840461	0.812113	–1.760222
H	–6.444669	–0.642073	–1.517835
O	5.513465	–0.827884	0.127427
H	5.764462	–1.763001	0.204801
H	6.311980	–0.277913	0.186592
O	1.903935	4.877138	0.885632
H	1.478482	4.394968	0.129002
H	2.788097	5.185573	0.633669
O	1.845622	–3.267810	1.774526
H	2.043208	–2.580104	1.093674
H	2.510039	–3.299975	2.476739
O	–1.447579	–2.034939	–3.555545
H	–2.301533	–2.233951	–3.972858
H	–0.726753	–2.385196	–4.103333

trans–$[Ru(H_2O)(NH_3)_4(P(OEt)_3)]^{2+}$ + NO + $8H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	0.988243	–0.654137	–0.134391
N	1.631488	0.046957	1.779598
H	2.653526	0.043113	1.808438
H	1.303225	0.988675	1.972585
H	1.280165	–0.581264	2.510660
P	–1.049433	0.183686	0.013040
N	1.780635	1.095562	–1.055446
H	2.731542	0.866787	–1.335417

H	1.269441	1.427610	–1.874302
H	1.800412	1.888151	–0.410594
N	0.527883	–1.460839	–2.054277
H	1.389431	–1.699057	–2.547438
H	–0.046291	–2.307306	–1.934176
H	–0.003758	–0.789350	–2.602071
N	0.570604	–2.552369	0.709461
H	1.457181	–3.042500	0.601528
H	0.349935	–2.509104	1.705746
H	–0.148981	–3.054580	0.176161
O	2.925952	–1.470091	–0.367696
H	3.220790	–1.774640	–1.269377
H	3.658399	–1.148822	0.228059
N	6.158481	2.044360	0.493232
O	7.197269	2.566211	0.672242
O	–2.437296	–0.652267	0.672661
C	–2.432146	–1.114791	2.068615
H	–1.870963	–0.402092	2.677076
H	–1.926119	–2.080320	2.106622
C	–3.861813	–1.229738	2.541728
H	–4.418063	–1.938506	1.926443
H	–4.364280	–0.262875	2.505517
H	–3.875830	–1.589689	3.572724
O	–1.249978	1.688669	0.873626
C	–2.502911	2.155522	1.505861
H	–2.446354	1.881572	2.560486
H	–3.352856	1.644935	1.055536
C	–2.618312	3.653725	1.344500
H	–2.637528	3.939894	0.291808
H	–1.799553	4.179363	1.837973
H	–3.552751	3.986570	1.802501
O	–1.749707	0.477360	–1.503104
C	–2.969097	1.261320	–1.738865
H	–2.726425	2.314640	–1.578801
H	–3.744249	0.966687	–1.030526
C	–3.399056	1.016398	–3.165338
H	–3.639781	–0.035971	–3.323432
H	–2.613434	1.304709	–3.865497
H	–4.289773	1.609554	–3.385152
O	–1.201335	–3.666053	–1.313705
H	–1.179150	–4.595561	–1.584754
H	–2.145437	–3.318588	–1.233473
O	3.425092	–2.231442	–2.815266
H	3.901144	–1.663345	–3.441127
H	3.553883	–3.165919	–3.041632
O	0.649216	3.414277	0.280945
H	–0.095072	2.837345	0.615997
H	0.898632	4.103993	0.912759
O	4.622659	–0.482458	1.345969
H	5.185221	0.280077	1.119049
H	5.050660	–1.034486	2.018758
O	–5.667569	1.280860	0.348338
H	–6.166870	0.488734	0.606816
H	–6.285195	2.020810	0.227122
O	0.519762	3.447498	–2.373321
H	0.533188	3.597304	–1.388146
H	–0.281513	3.822514	–2.769648
O	–3.467984	–2.512869	–0.897391
H	–3.204132	–1.724948	–0.347373
H	–4.198397	–2.314580	–1.499983
O	0.653131	–2.030011	3.645082
H	1.340167	–2.586840	4.047128

H	–0.042713	–1.853725	4.298996

trans–[Ru(H_2O)(NH_3)$_4$(P(OEt)$_3$)]$^{2+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.920229	0.677285	–0.246905
N	–0.755283	1.024370	–2.350363
H	–1.283127	1.846634	–2.635635
H	0.227091	1.188148	–2.569438
H	–1.074214	0.242701	–2.917450
P	1.156443	–0.099756	–0.163873
N	–0.144871	2.636793	0.038069
H	–0.887994	3.305507	–0.154583
H	0.185469	2.795806	0.986818
H	0.634213	2.820414	–0.591055
N	–1.107000	0.445457	1.872116
H	–1.501211	1.269460	2.321120
H	–1.686657	–0.349440	2.130359
H	–0.170118	0.295591	2.249664
N	–1.941097	–1.170651	–0.533516
H	–2.927592	–0.989983	–0.353956
H	–1.863341	–1.538296	–1.478435
H	–1.630164	–1.899040	0.104067
O	–2.878588	1.574015	–0.305811
H	–3.372346	1.875995	0.470274
O	1.741265	–1.683322	–0.453697
C	1.568915	–2.329589	–1.758467
H	2.059448	–1.724602	–2.524822
H	0.503417	–2.390830	–1.991514
C	2.184265	–3.704557	–1.670797
H	1.693401	–4.300356	–0.900412
H	3.248342	–3.638937	–1.440463
H	2.070312	–4.217764	–2.628050
O	2.121036	0.830207	–1.225823
C	3.561197	0.657566	–1.459117
H	3.673922	0.505082	–2.533012
H	3.908544	–0.243715	–0.948792
C	4.305773	1.890392	–1.001726
H	4.188216	2.051262	0.071217
H	3.942567	2.775169	–1.526329
H	5.370845	1.777342	–1.216970
O	1.799008	0.061163	1.397031
C	3.055825	–0.513632	1.896456
H	3.877841	0.122182	1.561908
H	3.178796	–1.510958	1.475501
C	2.973586	–0.545636	3.403343
H	2.152427	–1.183177	3.734113
H	2.825533	0.456862	3.807163
H	3.905164	–0.944974	3.810743
H	–3.410647	1.667996	–1.109453

trans–[Ru(H_2O)(NH_3)$_4$(P(OEt)$_3$)]$^{+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–1.026143	0.661972	–0.230223
N	–0.749251	1.388261	–2.233171
H	–1.124023	2.323780	–2.368630
H	0.268957	1.409629	–2.337379
H	–1.143668	0.785169	–2.949703
P	0.984152	–0.392316	–0.336765
N	0.062902	2.349668	0.459766
H	–0.539389	3.137830	0.681501
H	0.591259	2.070094	1.284515
H	0.739002	2.618890	–0.252072
N	–1.247062	0.064041	1.819002
H	–1.700369	0.775042	2.387438

H	–1.749821	–0.809616	1.947982
H	–0.279205	–0.056992	2.130515
N	–2.299060	–0.924645	–0.909028
H	–3.238589	–0.532921	–0.930150
H	–2.056469	–1.250232	–1.840451
H	–2.292320	–1.730122	–0.289381
O	–3.021142	1.807754	–0.097680
H	–3.513686	1.912249	0.731583
O	2.391676	–1.912376	–0.479070
C	2.238238	–2.676563	–1.690144
H	2.894111	–2.277266	–2.477919
H	1.206420	–2.597548	–2.068131
C	2.570817	–4.139375	–1.444686
H	1.901927	–4.563358	–0.692101
H	3.598188	–4.247439	–1.089231
H	2.465559	–4.720606	–2.365966
O	1.905816	0.795676	–1.305185
C	3.302802	0.671444	–1.696265
H	3.331192	0.621553	–2.788976
H	3.699362	–0.264494	–1.297896
C	4.089300	1.868044	–1.199789
H	4.075856	1.918560	–0.109007
H	3.673652	2.798297	–1.592713
H	5.130336	1.794546	–1.526334
O	1.562446	–0.059968	1.306917
C	2.832046	–0.477337	1.880800
H	3.652127	–0.114528	1.256143
H	2.881680	–1.566280	1.894171
C	2.918780	0.102138	3.276886
H	2.096372	–0.259417	3.897833
H	2.878072	1.192919	3.250001
H	3.859267	–0.195232	3.747910
H	–3.263734	2.515257	–0.715418

Table S2. Experimental (Exp) and calculated (Cal) geometric parameters of the complex *trans*–$[RuCl(NO)(NH_3)_4]^{2+}$.

Complex	Exp	Cal	|(Cal–Exp)/Exp| (%)
Bond distances [Å]			
Ru–NO	1.799	1.740	3.3
N–O[a]	1.026	1.168	13.8
Ru–Cl	2.376	2.384	0.3
$Ru–NH_{3(cis)}$[b,c]	2.100	2.115	0.7
Bond angles [°]			
Ru–N–O	176.6	179.6	1.7
Cl–Ru–NO	177.9	179.7	1.0
$NH_{3(cis)}$–Ru–NO[c]	92.0	94.1	2.3
Cl–Ru–$NH_{3(cis)}$[c]	88.1	85.9	2.5

[a] Disorder problem observed in the experimental measure of this bond length (S. I. Gorelsky, S. C. da Silva, A. B. P. Lever and D. W. Franco, *Inorg. Chim. Acta*, 2000, **300**, 698–708); [b] Ru–$NH_{3(cis)}$ is the Ru–NH_3 chemical bond in *cis* position in relation to Ru–NO bond; [c] Average value.

Table S3. Ratio between kinetic energy density, G_b, and potential energy density, V_b, $-G_b/V_b$, and electron density, ρ_b, at the selected BCPs of the transition states: $[RuCl(HNO)(H_2O)(NH_3)_4]^{2+‡}$ + $8H_2O$, *trans*–$[RuCl(H_2O)(NH_3)_4]^{2+‡}$ + $HNO\cdots H_2O$ + $7H_2O$, $[Ru(HNO)(H_2O)_2(NH_3)_4]^{3+‡}$ + $8H_2O$ and $[Ru(H_2O)(NO)(NH_3)_4(P(OEt)_3)]^{2+‡}$ + $8H_2O$. The values of all the parameters are in a.u.

Complex	BCP	$-G_b/V_b$	ρ_b
$[RuCl(HNO)(H_2O)(NH_3)_4]^{2+‡}$ + $8H_2O$	OHN···Ru	0.874	0.058
	HNO···H–NH_2	1.242	0.018
	OHN···OH_2	0.994	0.045
	ONH···OH_2	0.865	0.045
trans–$[RuCl(H_2O)(NH_3)_4]^{2+‡}$ + $HNO\cdots H_2O$ + $7H_2O$	OHN···Ru	0.856	0.037
	OHN···Cl^-	1.049	0.024
	OHN···OH_2	1.348	0.006
	HNO···OH_2	1.525	0.003
	ONH···OH_2	0.808	0.052
$[Ru(HNO)(H_2O)_2(NH_3)_4]^{3+‡}$ + $8H_2O$	OHN···Ru	0.873	0.057
	OHN···OH_2	0.992	0.046
	HNO···H–NH_2	1.223	0.019
	ONH···OH_2	0.896	0.041
$[Ru(H_2O)(NO)(NH_3)_4(P(OEt)_3)]^{2+‡}$ + $8H_2O$	Ru–NO	0.840	0.056
	Ru–O_2H	0.970	0.024
	NH_2–H···NO	1.147	0.025
	NO···H–NH_2	1.279	0.016
	HO–H···OH_2	0.864	0.043
		0.827	0.049
	H_2O···H–NH_2	1.014	0.034
	H_2O···NO	1.117	0.017