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How the Acidic Milieu Interferes in the Capability of Ruthenium Nitrosyl Complexes to Release Nitric Oxide?

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Supplementary Material

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

$[Ru(NO)(NH_3)_5]^{3+}$ + H_2O (NIMAG = 0)

Atom	X	Y	Z
Ru	0.336569	–0.077897	0.005437
N	0.080617	–2.182623	–0.075493
N	1.808194	–0.382934	1.513002
N	–1.157968	–0.030345	–1.492132
N	1.838985	–0.287480	–1.488913
N	–1.162177	–0.090381	1.501684
H	0.586602	–2.667924	0.664235
H	–0.902088	–2.435628	0.022600
H	0.396059	–2.586861	–0.956638
H	1.386819	–0.608892	2.412481
H	2.464364	–1.127456	1.284527
H	2.360809	0.461861	1.647379
H	–1.131204	–0.850407	–2.094962
H	–1.056342	0.783491	–2.095280
H	–2.097916	0.014943	–1.057950
H	2.545107	0.441621	–1.401498
H	2.330452	–1.177791	–1.434302
H	1.447223	–0.213464	–2.426049
H	–1.063012	0.710012	2.123549
H	–1.125809	–0.923339	2.086049
H	–2.104246	–0.038606	1.073280
O	–3.540458	0.058354	0.006174
H	–4.053673	0.882640	0.021785
H	–4.139279	–0.706018	–0.012546
N	0.472932	1.661249	0.043944
O	0.529916	2.822931	0.054548

$[Ru(NO)(NH_3)_5]^{2+}$ + H_2O (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.342962	–0.146493	–0.001325
N	–0.036887	–2.176519	0.729873
N	–1.824014	–0.850406	–1.385149
N	1.126854	0.546142	1.362929
N	–1.838296	0.106426	1.504920
N	1.174729	–0.563422	–1.441649
H	–0.579445	–2.856861	0.202070
H	0.944676	–2.434974	0.653299
H	–0.292533	–2.274520	1.709957
H	–1.450099	–1.514771	–2.058656
H	–2.618450	–1.292048	–0.927939
H	–2.171030	–0.046944	–1.904383
H	1.096161	0.062220	2.257222
H	0.993441	1.539951	1.543602
H	2.069088	0.423509	0.965306
H	–2.620110	0.640378	1.133212
H	–2.209001	–0.778167	1.844497
H	–1.474978	0.615534	2.307519
H	1.027355	0.006075	–2.270816
H	1.174847	–1.536576	–1.738782
H	2.105558	–0.343017	–1.059178
O	3.602801	0.136066	–0.058288

H	4.098127	0.922645	–0.338746
H	4.219059	–0.561823	0.216982
N	–0.555984	1.580043	–0.586530
O	–0.256234	2.744576	–0.333302

$[Ru(H_2O)(NO)(NH_3)_5]^{2+}$ (NIMAG = 1)

Atom	X	Y	Z
Ru	0.000000	0.000000	0.000000
N	0.000000	0.000000	2.079922
N	2.124901	0.000000	–0.019339
N	–2.136464	0.163234	0.244370
N	0.244580	–2.123252	0.238729
N	–0.106492	2.126775	–0.056462
O	0.727904	0.570146	–2.253233
N	–1.053852	–1.077836	–1.745196
H	–0.194537	0.924334	2.460827
H	–0.695606	–0.640334	2.458898
H	0.907452	–0.283437	2.444677
H	2.527355	0.852740	0.364073
H	2.563688	–0.783034	0.458594
H	2.358405	–0.046453	–1.009896
H	–2.566744	–0.760000	0.262507
H	–2.529949	0.656989	–0.553854
H	–2.414095	0.658866	1.088178
H	0.806085	–2.481127	–0.531159
H	0.695843	–2.391772	1.109853
H	–0.657237	–2.595093	0.191009
H	–0.776077	2.529230	0.595395
H	–0.394249	2.392773	–0.995233
H	0.793810	2.565759	0.124893
H	0.149078	0.055902	–2.845900
H	1.086030	1.363360	–2.684483
O	–1.904233	–1.976113	–1.560002

$[Ru(H_2O)(NH_3)_5]^{2+}$ + NO (NIMAG = 0)

Atom	X	Y	Z
Ru	0.618992	–0.043075	–0.007893
N	2.289322	–0.162113	–1.297455
N	0.077925	1.886913	–0.761883
N	1.078150	–1.974442	0.801311
N	–0.605799	–0.991061	–1.499093
N	1.799349	0.927805	1.495237
H	3.146746	–0.290399	–0.763893
H	2.217994	–0.943669	–1.946125
H	2.396883	0.684023	–1.852978
H	0.853164	2.546354	–0.759461
H	–0.290835	1.852328	–1.709460
H	–0.649845	2.263357	–0.157046
H	1.792431	–1.935587	1.525214
H	1.409848	–2.622627	0.089716
H	0.240481	–2.375932	1.218459
H	–1.589512	–0.759487	–1.375514
H	–0.342966	–0.701451	–2.439145
H	–0.526680	–2.004936	–1.460125
H	2.507034	1.537664	1.091039
H	2.279589	0.276322	2.112663
H	1.189037	1.503815	2.072078
O	–1.063812	0.141360	1.342515
H	–1.986871	0.157204	1.037636
H	–1.011830	–0.134602	2.268974
N	–3.689269	0.227331	–0.181964
O	–4.849589	0.403255	–0.107951

$[Ru(NO)(NH_3)_5]^{2+}$ (NIMAG = 0)

Atom	X	Y	Z

Ru	–0.144127	–0.015822	0.014264
N	–1.049110	0.263368	–1.900446
N	1.484389	–0.433956	–0.729135
N	0.428877	2.033182	0.011495
N	0.630022	–0.200770	1.993771
N	–0.717793	–2.077202	0.003308
N	–2.061993	0.480088	0.921503
H	0.074730	0.306221	2.679619
H	0.674272	–1.172395	2.292268
H	1.577404	0.168787	2.035437
H	–1.617196	–2.237152	–0.445296
H	–0.013198	–2.598460	–0.514306
H	–0.774543	–2.478575	0.936604
H	–1.813527	0.935270	–1.883404
H	–0.356783	0.610696	–2.560244
H	–1.414298	–0.608161	–2.277557
H	0.415860	2.444446	0.942322
H	1.379531	2.118948	–0.347060
H	–0.171533	2.604487	–0.579251
H	–2.113123	1.457186	1.201464
H	–2.836760	0.305751	0.284679
H	–2.231017	–0.088145	1.749173
O	2.553826	0.053858	–1.079642

$[Ru(HNO)(NH_3)_5]^{3+}$ (NIMAG = 0)

Atom	X	Y	Z
Ru	–0.178421	–0.024390	–0.013694
N	–1.057299	0.293267	–1.916505
N	1.574504	–0.449674	–0.763454
N	0.405956	2.000365	0.029308
N	0.679141	–0.171610	1.907597
N	–0.735886	–2.071317	–0.019370
N	–2.082845	0.442858	0.862325
H	0.251638	0.463080	2.580739
H	0.590972	–1.110880	2.297450
H	1.677081	0.040943	1.870612
H	–1.689437	–2.213068	0.309534
H	–0.673853	–2.493418	–0.946657
H	–0.124733	–2.627139	0.579260
H	–1.752410	1.038973	–1.897683
H	–0.373005	0.531422	–2.632837
H	–1.543553	–0.543198	–2.241366
H	0.074082	2.497245	0.854621
H	1.425604	2.061165	0.019316
H	0.066522	2.519385	–0.781046
H	–2.189875	1.442257	1.030765
H	–2.866913	0.162447	0.275283
H	–2.214136	–0.018951	1.762000
O	2.640776	0.101891	–0.416633
H	1.726473	–1.178442	–1.484564

$[Ru(HNO)(NH_3)_5]^{3+} + H_2O$ (NIMAG = 0)

Atom	X	Y	Z
Ru	0.404159	0.075288	0.170497
N	0.509462	–0.129124	2.274486
N	2.543193	0.301235	–0.018106
N	0.632989	–2.023779	0.024612
N	0.232077	0.377008	–1.915461
N	0.220112	2.162921	0.478508
O	–2.616388	0.736170	–2.028133
N	–1.525943	–0.179670	0.258660
H	–3.109338	0.135846	–2.611500
H	–2.134919	0.159683	–0.548121
H	–2.989453	1.631738	–2.077835

O	–2.153260	–0.754329	1.173946
H	2.925458	–0.347714	–0.705292
H	2.817361	1.233593	–0.324169
H	3.028031	0.125386	0.860378
H	–0.475044	2.378369	1.192519
H	1.096045	2.600464	0.758536
H	–0.090900	2.627923	–0.374995
H	–0.740780	0.610275	–2.171430
H	0.847466	1.113981	–2.255264
H	0.481324	–0.463995	–2.436593
H	0.020760	–2.494480	0.691402
H	0.371310	–2.371767	–0.897866
H	1.586220	–2.334697	0.205492
H	–0.424743	–0.312177	2.643881
H	1.106151	–0.906825	2.555248
H	0.880252	0.698360	2.739765

$[Ru(HNO)(H_2O)(NH_3)_5]^{3+}$ (NIMAG = 1)

Atom	X	Y	Z
Ru	–0.059648	0.005953	–0.111377
N	–0.103568	0.055494	2.040483
N	2.004604	0.043535	0.087471
N	0.222167	–2.101893	–0.304259
N	0.181725	0.061894	–2.223963
N	–0.092898	2.137830	0.035451
O	–2.172113	0.592800	–0.988437
N	–2.199069	–1.103835	0.668215
H	–2.593823	0.140797	–1.738407
H	–3.008709	–0.520491	0.976225
H	–2.671695	1.395393	–0.764840
O	–2.537084	–2.256446	0.381699
H	2.463726	–0.664845	–0.482599
H	2.388324	0.945486	–0.196543
H	2.300121	–0.114474	1.049435
H	–0.864362	2.462163	0.615496
H	0.756363	2.518029	0.450192
H	–0.195291	2.572723	–0.879773
H	–0.310545	0.869262	–2.601224
H	1.152574	0.130945	–2.524389
H	–0.212015	–0.764777	–2.669750
H	–0.675560	–2.587861	–0.243674
H	0.642649	–2.361770	–1.194072
H	0.816530	–2.483060	0.430254
H	–0.982433	0.438939	2.381268
H	–0.011487	–0.876523	2.439892
H	0.633320	0.633933	2.440437

$[Ru(H_2O)(NH_3)_5]^{3+}$ + HNO (NIMAG = 0)

Atom	X	Y	Z
Ru	0.426182	0.314185	–0.218946
N	–0.082994	0.168614	1.824465
N	2.449026	0.107053	0.239383
N	0.216018	–1.788468	–0.421735
N	0.901348	0.457212	–2.283180
N	0.560132	2.429923	0.008663
O	–1.571814	0.513654	–0.694739
N	–2.621199	–1.462700	1.871323
H	–2.030934	–0.010115	–1.370885
H	–3.508378	–1.580925	2.419311
H	–2.165438	1.182719	–0.319468
O	–2.488717	–2.377935	1.045663
H	2.826212	–0.786521	–0.071249
H	3.012306	0.830044	–0.208685
H	2.622526	0.185549	1.240800

H	–0.178181	2.793021	0.609353
H	1.442861	2.721032	0.426262
H	0.474926	2.913056	–0.884355
H	0.069866	0.744388	–2.798953
H	1.622799	1.148048	–2.483770
H	1.219667	–0.424432	–2.680220
H	–0.686094	–2.086899	–0.036939
H	0.244184	–2.092862	–1.392563
H	0.933348	–2.312979	0.076593
H	–1.041337	–0.204278	1.912459
H	0.520885	–0.470918	2.338473
H	–0.046948	1.065529	2.303219

$[Ru(HNO)(NH_3)_5]^{3+}$ + $9H_2O$ (NIMAG = 0)

Atom	X	Y	Z
O	2.304080	3.383267	–1.498488
H	3.269254	3.361892	–1.598195
H	1.963807	4.260800	–1.735355
O	–3.084903	–2.802620	2.325875
H	–2.421085	–3.065715	1.651158
H	–3.787996	–3.460350	2.422696
O	–2.600895	–0.268777	2.219743
H	–3.197160	0.476415	1.995207
H	–3.039183	–1.133668	2.450070
O	–1.832925	1.345932	–3.167241
H	–2.279086	0.649543	–3.674656
H	–1.980728	2.212139	–3.578907
O	–3.481466	1.936497	0.934177
H	–4.337057	1.933183	0.473862
H	–3.352684	2.786259	1.386969
O	2.756357	–1.030412	–3.217270
H	2.567104	–1.356328	–4.112998
H	3.717204	–0.946420	–3.103827
O	1.441858	–2.875724	1.644334
H	0.612306	–3.236262	1.269307
H	1.905819	–3.522336	2.196630
O	1.998762	1.715527	3.147070
H	1.623964	2.257253	3.860172
H	2.940751	1.553346	3.316020
Ru	0.352079	0.054400	–0.222410
N	0.243423	–0.234681	1.915907
N	2.274461	–0.682498	0.145578
N	0.429556	–1.580664	–1.612828
N	0.924116	0.935445	–2.079544
N	0.878858	1.971015	0.520367
O	–1.461801	1.120196	–0.616403
N	–1.142237	–1.292187	0.203356
H	–1.726104	1.229202	–1.575145
H	–1.902926	–0.842173	0.765106
H	–2.188372	1.388037	0.010934
O	–0.994498	–2.579259	0.442054
H	2.791222	–0.855819	–0.712939
H	2.818953	–0.024589	0.698233
H	2.186142	–1.568305	0.675320
H	–0.006608	2.470805	0.577109
H	1.332673	1.984599	1.442885
H	1.479898	2.491716	–0.136428
H	0.084898	1.051388	–2.656904
H	1.349332	1.863289	–1.948298
H	1.605949	0.361606	–2.589897
H	–0.344432	–1.511844	–2.269478
H	1.312622	–1.588695	–2.135271
H	0.310502	–2.451238	–1.092737

H	–0.723945	–0.117208	2.251584
H	0.558183	–1.191042	2.111266
H	0.864741	0.409734	2.418511

$[Ru(HNO)(H_2O)(NH_3)_5]^{3+}$ + 8H_2O (NIMAG = 1)

Atom	X	Y	Z
O	2.894425	3.162605	4.469015
H	3.854268	3.016857	4.461284
H	2.694368	4.059789	4.156715
O	–2.687234	–4.068126	8.486961
H	–2.225750	–3.650705	7.732469
H	–3.561445	–4.381288	8.205568
O	–2.502522	–0.013122	8.044196
H	–2.815986	0.875945	7.728702
H	–3.037427	–0.361684	8.772442
O	–1.552650	0.971754	2.634678
H	–1.846493	0.166198	2.180960
H	–1.838025	1.759894	2.146399
O	–2.963466	2.245507	6.771277
H	–3.823199	2.348096	6.330270
H	–2.701867	3.083578	7.187326
O	2.774971	–1.351003	2.528017
H	2.477117	–1.606373	1.639749
H	3.733349	–1.486581	2.601968
O	2.351812	–3.282458	6.621120
H	2.072819	–3.694593	7.454871
H	2.977715	–3.867961	6.163981
O	2.021965	1.580913	9.171753
H	1.520335	1.999117	9.890584
H	2.963111	1.547750	9.407576
Ru	0.708168	0.098005	5.678139
N	0.401972	–0.375175	7.766084
N	2.667613	–0.493916	6.123608
N	0.794313	–1.770263	4.620505
N	1.272306	0.830541	3.770140
N	1.140852	2.025519	6.434901
O	–1.141113	1.013594	5.182797
N	–1.353604	–1.479222	6.100898
H	–1.423287	1.005718	4.223643
H	–1.969551	–0.943192	6.795700
H	–1.780294	1.477901	5.776518
O	–1.300667	–2.716685	6.324634
H	3.284031	–0.385749	5.321092
H	3.064488	0.051654	6.884570
H	2.665182	–1.490391	6.398571
H	0.294815	2.584874	6.362828
H	1.461479	2.022408	7.410350
H	1.856097	2.478585	5.846336
H	0.429022	0.997413	3.216387
H	1.789490	1.712567	3.870111
H	1.865952	0.169127	3.256650
H	–0.090976	–1.940686	4.155392
H	1.538906	–1.751700	3.913836
H	0.983728	–2.531199	5.276489
H	–0.549881	–0.152036	8.079528
H	0.577659	–1.356831	7.963636
H	1.054103	0.186352	8.328064

$[Ru(H_2O)(NH_3)_5]^{3+}$ + HNO + 8H_2O (NIMAG = 0)

Atom	X	Y	Z
O	2.778164	3.364056	–1.636657
H	3.745253	3.279878	–1.607965
H	2.536986	4.200043	–2.068252
O	–5.504947	–3.323319	1.648887

H	–4.730947	–3.306973	1.049654
H	–6.275194	–2.936725	1.203190
O	–2.349005	–0.754989	2.408806
H	–2.741111	0.128343	2.185594
H	–2.607053	–1.049956	3.295289
O	–1.957330	0.789831	–2.827549
H	–2.097553	–0.015107	–3.349738
H	–2.478990	1.525323	–3.184174
O	–2.992686	1.622632	1.388333
H	–3.881259	1.734604	1.011009
H	–2.754286	2.404852	1.912990
O	1.619398	–1.492973	–3.530869
H	1.072969	–1.648680	–4.318137
H	2.493974	–1.896364	–3.653785
O	2.987761	–2.681632	0.602716
H	3.020377	–3.069037	1.492444
H	3.540001	–3.205059	–0.000948
O	1.416527	2.225684	3.353098
H	0.810485	2.713569	3.933958
H	2.301706	2.198461	3.751166
Ru	0.783373	0.422865	–0.130957
N	0.505436	–0.151812	1.898313
N	2.838395	0.111713	0.104019
N	0.609187	–1.579353	–0.781331
N	1.074827	1.011081	–2.146905
N	1.018420	2.434394	0.485427
O	–1.215397	0.737630	–0.389473
N	–2.179826	–2.457484	0.205601
H	–1.595117	0.727920	–1.325063
H	–2.350122	–1.882327	1.090284
H	–1.846718	1.098000	0.288865
O	–3.146220	–3.206827	–0.038400
H	3.353729	0.313168	–0.749885
H	3.232412	0.680789	0.849327
H	2.997737	–0.884582	0.338772
H	0.139122	2.921107	0.323607
H	1.248826	2.509564	1.483567
H	1.735012	2.890898	–0.093786
H	0.176557	1.276911	–2.552467
H	1.709633	1.816203	–2.188234
H	1.441216	0.234433	–2.709112
H	–0.344442	–1.919941	–0.614023
H	0.833663	–1.654002	–1.780101
H	1.263115	–2.175871	–0.264065
H	–0.475927	–0.394083	2.092120
H	1.067653	–0.965831	2.135190
H	0.782504	0.617732	2.520090

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*–$[Ru(H_2O)(NH_3)_5]^{3+}$ (NIMAG = 0)**

Atom	X	Y	Z
Ru	–0.049249	0.028586	–0.022755
N	0.050353	0.012058	2.106176
O	2.005220	0.086600	–0.080566
N	–0.010997	–2.088019	0.019510
N	–0.082672	0.004518	–2.149842
N	–0.063609	2.140245	–0.071445
N	–2.129386	0.047873	0.047521
H	–1.009416	–0.204624	–2.518683
H	0.205438	0.892935	–2.556284
H	0.545791	–0.705970	–2.523854
H	–0.392078	2.522186	–0.956284
H	–0.630406	2.559711	0.663827
H	0.894490	2.464355	0.064532
H	–0.837701	–0.231633	2.541817
H	0.732867	–0.664781	2.445419
H	0.325609	0.918997	2.480142
H	–0.496816	–2.516174	–0.767250
H	0.963374	–2.386858	–0.034540
H	–0.402651	–2.482355	0.872865
H	–2.501830	–0.893226	–0.079174
H	–2.484116	0.383004	0.942316
H	–2.539790	0.634108	–0.677188
H	2.518337	0.333624	–0.866061
H	2.591571	–0.079491	0.674796

***trans*–$[Ru(H_2O)(NH_3)_5]^{2+}$ (NIMAG = 0)**

Atom	X	Y	Z
Ru	–0.064878	0.026810	–0.020157
N	0.012286	0.030952	2.126526
O	2.103369	–0.050352	–0.080817
N	0.015216	–2.108658	–0.004059
N	–0.117063	–0.007882	–2.168620
N	–0.021845	2.169269	–0.038756
N	–2.175308	0.042095	0.036385
H	–1.039902	–0.263895	–2.513729
H	0.121864	0.893481	–2.576918
H	0.541907	–0.690987	–2.537721
H	–0.467140	2.559237	–0.866761
H	–0.489776	2.571512	0.770472
H	0.945773	2.486056	–0.028739
H	–0.877789	–0.245746	2.536511
H	0.712816	–0.624742	2.467699
H	0.247689	0.947891	2.501057
H	–0.443223	–2.536215	–0.805573
H	1.002004	–2.359434	–0.032122
H	–0.392836	–2.514539	0.834839
H	–2.561406	–0.889657	–0.100782
H	–2.525323	0.388195	0.927724
H	–2.561749	0.644444	–0.687880
H	2.594773	0.171596	–0.885510
H	2.642874	0.136239	0.701927

Table S2. Experimental geometric parameters to $[Ru(NO)(NH_3)_5]^{3+}$ and theoretical geometric parameters to $[Ru(NO)(NH_3)_5]^{3+}$ complex explicitly solvated from one H_2O molecule, $[Ru(NO)(NH_3)_5]^{3+} + H_2O$, along with the PCM($H_2O$) method.

	Experimental	Theoretical
Bond distances [Å]		
Ru–NO	1.771	1.745
N–O	1.172	1.163
$Ru–NH_{3(trans)}$[a]	2.017	2.122
$Ru–NH_{3(cis)}$[b,c]	2.093	2.123
Bond angles [º]		
Ru–N–O	172.9	178.2
$NH_{3(trans)}$–Ru–NO	175.4	177.4
$NH_{3(cis)}$–Ru–NO[c]	90.8	93.3
$NH_{3(trans)}$–Ru–$NH_{3(cis)}$[c]	89.3	86.8

[a] $Ru–NH_{3(trans)}$ is the Ru–NH_3 chemical bond in *trans* position in relation to Ru–NO bond. [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. The electronic energy (Δ*E*) to selected complexes studied in this paper with the PBE0–D3(BJ)/Def2–TZVP computational model. The energy values are in Hartree.

Complex	Δ*E*
$[Ru(NO)(NH_3)_5]^{2+} + H_2O$	–583.62
$[Ru(H_2O)(NO)(NH_3)_5]^{2+}$	–583.55
$[Ru(H_2O)(NH_3)_5]^{2+} + NO$	–583.57
$[Ru(HNO)(NH_3)_5]^{3+} + H_2O$	–584.00
$[Ru(HNO)(H_2O)(NH_3)_5]^{3+}$	–583.95
$[Ru(H_2O)(NH_3)_5]^{3+} + HNO$	–583.97
$[Ru(HNO)(NH_3)_5]^{3+} + 9H_2O$	–1195.15
$[Ru(HNO)(H_2O)(NH_3)_5]^{3+} + 8H_2O$	–1195.14
$[Ru(H_2O)(NH_3)_5]^{3+} + HNO + 8H_2O$	–1195.15

Table S4. Electron density, ρ_b, Laplacian of ρ_b, $\nabla^2\rho_b$, and $-G_b/V_b$, at the selected BCPs of $[Ru(HNO)(H_2O)(NH_3)_5]^{3+} + 8H_2O$. The values of all the parameters are in a.u.

BCP	ρ_b	$\nabla^2\rho_b$	$-G_b/V_b$
HNO···H_2O	0.024	0.088	1.078
H_2O···HNO	0.055	0.131	0.792