ARTICLE

Are the Relative Positions (*cis*–*trans*) of Ligands Really Able to Modulate the Coordination of NO in Ruthenium Nitrosyl Complexes?

Renato Pereira Orenha,*[a] Graziele Cappato Guerra Silva,[a] Nelson Henrique Morgon,[b] 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 of the compounds investigated in this paper from the ZORA–BP86/TZ2P computational model.

Complex		**1**	
Atom	X	Y	Z
Ru	–0.085026	0.002717	0.002464
N	–2.267673	0.064570	–0.013198
N	–0.135188	1.540893	1.554798
N	–0.236956	–1.544638	–1.532433
N	–0.185492	–1.533109	1.554905
N	–0.101024	1.559741	–1.529820
H	–2.675688	0.894934	0.440770
H	–2.674358	0.063481	–0.960229
H	–2.722861	–0.732099	0.455870
H	–0.550732	2.434737	1.257399
H	–0.658476	1.269691	2.398953
H	0.800885	1.793851	1.901882
H	–1.021785	–2.196660	–1.395552
H	0.597634	–2.146362	–1.580251
H	–0.353464	–1.188139	–2.491311
H	0.581019	–1.449361	2.237863
H	–1.041847	–1.522671	2.125845
H	–0.111858	–2.497546	1.201721
H	0.419323	2.402719	–1.247790
H	–1.032942	1.902609	–1.800374
H	0.343496	1.271309	–2.412989
N	1.690556	–0.049421	–0.018076
O	2.826494	–0.082934	–0.043370
Complex		**2**	
Atom	X	Y	Z
Ru	–0.114258	–0.002586	–0.016504
N	–2.206383	0.056649	0.958824
N	0.870977	0.224873	1.896480
N	–1.037161	–0.237865	–1.989405
N	–0.087731	–2.169284	0.256690
N	–0.188927	2.170985	–0.215447
H	–2.205158	0.233974	1.969103
H	–2.821678	0.777919	0.565717
H	–2.737073	–0.814512	0.846606
H	0.665915	1.095446	2.400152
H	0.692917	–0.522324	2.577346
H	1.891655	0.226207	1.756102
H	–1.633921	–1.063935	–2.110046
H	–0.290779	–0.331999	–2.689441
H	–1.614829	0.547662	–2.309342
H	0.849469	–2.500103	0.514601
H	–0.713925	–2.531623	0.984154

H	–0.320757	–2.696788	–0.592310
H	0.703109	2.605185	0.049090
H	–0.901237	2.644208	0.351236
H	–0.350097	2.486483	–1.178688
N	1.568165	–0.046858	–0.766201
O	2.705425	–0.007157	–0.438285

Complex		**3**	
Atom	X	Y	Z
Ru	–0.074151	0.002286	–0.253893
N	–1.028545	1.931339	–0.019937
N	1.001146	–1.844398	–0.614307
N	–2.139868	–1.074698	–0.475344
H	–1.220992	2.427514	–0.897041
H	–1.923135	1.897713	0.482645
H	–0.423109	2.561919	0.518645
H	0.746829	–2.345857	–1.472528
H	0.875102	–2.526330	0.142489
H	2.012117	–1.673621	–0.668161
H	–2.632353	–1.063277	0.425312
H	–2.807076	–0.671756	–1.142593
H	–2.083822	–2.068346	–0.725362
N	0.203136	–0.124331	1.471770
O	0.479221	–0.159391	2.585259
N	–0.039916	0.361052	–2.407162
H	0.387716	1.271608	–2.612827
H	0.539064	–0.310755	–2.924253
H	–0.951107	0.356854	–2.880581
H	1.313392	0.765258	–0.341099

Complex		**4**	
Atom	X	Y	Z
Ru	–0.162574	–0.379021	–0.093936
N	–2.289383	–0.407403	0.769541
H	0.290894	–0.246790	1.439020
N	–1.072971	–0.535657	–2.251278
N	0.007712	–2.551708	0.149806
N	–0.110617	1.769137	–0.159359
H	–1.428237	–1.458583	–2.515685
H	–0.313396	–0.337348	–2.908404
H	–1.821626	0.122900	–2.483246
H	0.983288	–2.770817	–0.078565
H	–0.126715	–2.845415	1.120618
H	–0.571526	–3.167866	–0.427959
H	0.857115	2.013306	–0.415688
H	–0.271077	2.189317	0.760056
H	–0.718582	2.261877	–0.820699

N	1.573093	–0.294768	–0.626838
O	2.421413	0.519742	–0.880149
H	–2.854461	0.420938	0.565408
H	–2.183847	–0.430910	1.787138
H	–2.874166	–1.211622	0.523030

Complex		**5**	
Atom	X	Y	Z
Ru	–0.028368	–0.028937	–0.038685
N	–0.223868	–1.499326	–1.580012
N	–0.281669	–1.564249	1.494055
N	0.005881	1.566886	–1.529166
H	0.163328	–2.417562	–1.317020
H	0.272424	–1.247243	–2.447415
H	–1.196110	–1.684409	–1.865441
H	–0.925721	–1.284411	2.248079
H	–0.649350	–2.463999	1.152934
H	0.596541	–1.808080	1.974759
H	0.943631	1.968955	–1.673179
H	–0.589498	2.369917	–1.279509
H	–0.305391	1.289931	–2.471233
N	1.747551	–0.194399	–0.040722
O	2.878417	–0.288372	–0.029630
N	–2.182646	0.214610	0.009297
H	–2.615931	0.546445	–0.865024
H	–2.723127	–0.625274	0.263796
H	–2.433274	0.921231	0.718923
O	–0.082134	1.478099	1.517700
H	0.250619	2.390830	1.373185
H	0.148550	1.274367	2.450421

Complex		**6**	
Atom	X	Y	Z
Ru	–0.053675	0.011697	0.004069
N	–0.076155	1.504248	1.588061
N	–0.030469	–1.496590	–1.547263
N	0.052798	1.518071	–1.516060
H	–0.464446	2.424732	1.352406
H	–0.599361	1.194673	2.415388
H	0.880022	1.686971	1.916223
H	–0.459584	–2.391765	–1.286131
H	0.938902	–1.729872	–1.804434
H	–0.488309	–1.230966	–2.426762
H	0.405705	2.417295	–1.168133
H	–0.840494	1.729568	–1.975268
H	0.701362	1.259771	–2.269995
N	1.778439	–0.138509	0.034648

O	2.690473	–0.410252	–0.664199
N	–2.341391	0.017641	0.035105
H	–2.773718	0.941419	0.147857
H	–2.811621	–0.395099	–0.777501
H	–2.667028	–0.527798	0.842022
O	–0.310622	–1.510817	1.627932
H	0.380630	–1.501460	2.320529
H	–0.447061	–2.459819	1.435287

Complex		**7**	
Atom	X	Y	Z
Ru	–0.133096	0.050088	0.023800
N	–0.221589	–1.955990	1.148307
N	–0.435731	–0.902085	–1.893052
N	–0.057964	1.184575	1.862518
H	–1.156627	–2.276754	1.420854
H	0.181540	–2.727888	0.605512
H	0.323589	–1.942248	2.017545
H	–0.802956	–1.859910	–1.868356
H	–1.092164	–0.353695	–2.462340
H	0.428160	–0.951546	–2.445309
H	–0.342510	0.685678	2.712839
H	–0.663696	2.011737	1.794459
H	0.881138	1.550163	2.057948
N	1.610307	–0.052033	–0.094684
O	2.760065	–0.113558	–0.175782
N	–2.345390	0.077575	0.231765
H	–2.577165	0.965178	–0.237989
H	–2.876459	–0.663096	–0.240423
H	–2.732837	0.126708	1.181010
N	–0.503407	1.775295	–0.897348
H	–0.088471	2.611388	–0.472235
H	–0.230783	1.826906	–1.884739

Complex		**8**	
Atom	X	Y	Z
Ru	–0.059893	0.029092	0.028358
N	–0.034857	1.468892	1.666073
N	–0.007325	–1.533659	–1.435107
N	–0.196458	1.660964	–1.552760
H	–0.468116	2.383664	1.511162
H	–0.485902	1.073723	2.497972
H	0.942345	1.647266	1.920631
H	–0.437937	–2.396458	–1.085041
H	0.986200	–1.752058	–1.600654
H	–0.427005	–1.353576	–2.352019
H	0.159629	2.560719	–1.218729

H	–1.147256	1.836460	–1.887985
H	0.366043	1.443471	–2.380204
N	1.751018	–0.003667	–0.072173
O	2.621334	–0.665824	–0.582807
N	–2.404871	–0.010450	0.069080
H	–2.967090	0.789355	0.372726
H	–2.915838	–0.443659	–0.704024
H	–2.366383	–0.696673	0.841161
N	–0.419776	–1.392204	1.421835
H	0.038001	–1.235586	2.326241
H	–0.116792	–2.339544	1.167817

Complex		**9**	
Atom	X	Y	Z
Ru	–0.050177	0.004374	0.001887
N	–0.083639	1.533980	1.573156
N	–0.239791	–1.507577	–1.574717
N	–0.320945	–1.562761	1.530808
H	–0.719779	2.316690	1.363533
H	–0.361524	1.191933	2.503802
H	0.834055	1.981439	1.713631
H	–0.546764	–2.435121	–1.249594
H	0.646079	–1.676386	–2.073527
H	–0.903084	–1.239329	–2.315849
H	0.140713	–1.343309	2.425803
H	–1.298019	–1.770010	1.781967
H	0.080126	–2.472266	1.258401
N	1.748628	–0.148307	0.060521
O	2.874319	–0.223485	0.078119
N	–2.218188	0.200122	–0.078651
H	–2.558635	0.907997	–0.747290
H	–2.702394	–0.668539	–0.350851
H	–2.643305	0.467656	0.821793
C	0.082336	1.432800	–1.384798
O	0.162102	2.241877	–2.170461

Complex		**10**	
Atom	X	Y	Z
Ru	–0.144913	0.112637	0.103288
N	–0.370580	1.335161	1.898382
N	–0.013788	–1.096022	–1.710276
N	–0.381909	–1.760756	1.342314
H	–1.219363	1.911607	1.907191
H	–0.373866	0.805320	2.777144
H	0.405448	2.001801	1.986374
H	0.045627	–2.107111	–1.545618
H	0.828527	–0.858469	–2.247346

H	–0.793664	–0.956279	–2.362238
H	0.542650	–2.087696	1.649742
H	–0.932282	–1.658150	2.202686
H	–0.805969	–2.562004	0.860810
N	1.716647	–0.014415	0.373220
O	2.737702	0.492010	0.131861
C	0.035502	1.679472	–0.934690
O	0.160296	2.630327	–1.563101
N	–2.417800	0.141267	–0.139571
H	–2.748358	0.936483	–0.697387
H	–2.797063	–0.691894	–0.603996
H	–2.929993	0.200718	0.748021

Complex		**11**	
Atom	X	Y	Z
Ru	0.000212	0.011203	–0.012948
N	–0.088581	1.556580	1.508969
N	–0.083852	–1.683791	–1.367692
N	–0.191244	1.504603	–1.711296
H	–0.922696	2.153976	1.493472
H	–0.076424	1.098801	2.430873
H	0.712407	2.198623	1.498435
H	–0.338369	–2.522028	–0.827573
H	0.824204	–1.899684	–1.795266
H	–0.744764	–1.614480	–2.149663
H	–0.049861	2.480163	–1.424656
H	–1.091285	1.498023	–2.204356
H	0.511502	1.341544	–2.441982
N	1.764019	–0.016250	0.034778
O	2.901175	–0.078597	0.122694
C	–0.140450	–1.302701	1.471211
N	–0.348909	–2.059073	2.337901
N	–2.180495	–0.081498	0.098864
H	–2.675133	0.818569	0.087490
H	–2.624624	–0.646754	–0.634872
H	–2.430079	–0.546014	0.983951

Complex		**12**	
Atom	X	Y	Z
Ru	–0.068719	–0.029554	–0.007285
N	–0.321294	–1.637874	–1.642519
N	–0.224757	–1.483917	1.613665
N	0.014575	1.611733	–1.430272
H	–0.856648	–2.467758	–1.372629
H	0.618718	–1.974782	–1.873752
H	–0.730937	–1.323263	–2.526556
H	–0.035279	–0.980000	2.487257

H	–1.128974	–1.949019	1.730229
H	0.477886	–2.224445	1.544664
H	0.173429	2.467854	–0.886765
H	–0.819703	1.770968	–2.002009
H	0.799333	1.531087	–2.082105
N	1.755366	–0.227250	–0.084785
O	2.785421	0.277353	0.210630
N	–2.345305	0.287995	0.160472
H	–2.604836	1.215272	–0.187614
H	–3.003840	–0.373436	–0.261972
H	–2.562441	0.332602	1.161066
C	0.025964	1.347104	1.384773
N	–0.022732	2.176465	2.213732

Complex		$[Ru(NH_3)_5]^{2+}$	
Atom	X	Y	Z
Ru	–0.164119	0.005016	0.005174
N	–2.244691	0.072732	0.002525
N	–0.010906	1.526226	1.545795
N	–0.112008	–1.524556	–1.535960
N	–0.117297	–1.539187	1.530338
N	–0.004379	1.539915	–1.522831
H	–2.622171	1.018060	0.142099
H	–2.663758	–0.257327	–0.875668
H	–2.674730	–0.500735	0.738680
H	–0.444182	2.432063	1.328643
H	–0.402548	1.271674	2.460448
H	0.971808	1.756036	1.743732
H	–0.685381	–2.358269	–1.358744
H	0.840173	–1.891820	–1.662484
H	–0.390822	–1.217823	–2.475724
H	0.849911	–1.772842	1.790172
H	–0.568797	–1.303645	2.422660
H	–0.533000	–2.439848	1.263685
H	–0.229142	2.494238	–1.217078
H	–0.581167	1.400493	–2.361216
H	0.956949	1.608998	–1.881559

Complex		$[RuH(NH_3)_4]^{+}$	
Atom	X	Y	Z
Ru	–0.918946	–0.284659	–0.345668
N	–1.721489	–0.106516	1.640421
H	0.522433	–0.112941	0.247453
N	–0.077846	–0.463297	–2.327037
N	–0.759800	–2.414409	–0.071492
N	–1.046419	1.849729	–0.614848
H	–0.690857	–0.902060	–3.023414

H	0.780337	–1.023190	–2.316747
H	0.204876	0.429636	–2.746052
H	0.179612	–2.750672	–0.305390
H	–0.905550	–2.723730	0.896857
H	–1.408987	–2.977897	–0.632145
H	–0.202100	2.223815	–1.061593
H	–1.119116	2.372295	0.264020
H	–1.834135	2.172556	–1.188481
H	–1.178932	0.565094	2.193181
H	–1.689377	–0.973075	2.190459
H	–2.698028	0.205212	1.692182

Complex		$[Ru(H_2O)(NH_3)_5]^{2+}$	
Atom	X	Y	Z
Ru	–0.177933	0.009846	–0.011163
N	–0.010383	1.502599	1.554704
N	–0.152220	–1.521126	–1.548431
N	–0.008853	1.521263	–1.494802
H	–0.277967	2.460210	1.295850
H	–0.557944	1.307742	2.402038
H	0.959208	1.591441	1.886218
H	–0.762059	–2.329641	–1.374479
H	0.787886	–1.923937	–1.657545
H	–0.406403	–1.212246	–2.494737
H	–0.363865	2.444806	–1.218303
H	–0.488888	1.319125	–2.380353
H	0.971079	1.688933	–1.761630
N	–2.244775	0.021462	0.081238
H	–2.658508	0.921452	0.352852
H	–2.716530	–0.243798	–0.791720
H	–2.554739	–0.658725	0.789603
O	–0.312314	–1.554241	1.531397
H	0.050846	–1.402793	2.425048
H	–0.080151	–2.480470	1.327546

Complex		$[Ru(NH_2)(NH_3)_5]^{+}$	
Atom	X	Y	Z
Ru	–0.212449	0.055826	0.013451
N	–0.157283	1.473105	1.634930
N	–0.128859	–1.522902	–1.451105
N	–0.085164	1.682245	–1.561553
H	–0.728532	2.320022	1.544202
H	–0.473263	1.012872	2.497271
H	0.790378	1.807084	1.839425
H	–0.453971	–2.399240	–1.024909
H	0.825878	–1.717351	–1.770577
H	–0.681105	–1.405485	–2.307140

H	0.322306	2.555152	–1.213156
H	–0.986360	1.952423	–1.967143
H	0.501545	1.425651	–2.361192
N	–2.255085	–0.074134	0.122114
H	–2.772315	0.736520	0.474873
H	–2.762407	–0.409781	–0.701989
H	–2.244874	–0.828012	0.855897
N	–0.412673	–1.402519	1.427842
H	–0.027413	–1.198420	2.357045
H	–0.021636	–2.323316	1.198248

Complex		$[Ru(CO)(NH_3)_4]^{2+}$	
Atom	X	Y	Z
Ru	–0.336623	0.122219	0.068403
N	–0.394149	1.363787	1.847908
N	–0.053803	–1.155682	–1.66355
N	–0.276172	–1.696751	1.378054
H	–0.820685	2.285719	1.7006
H	–0.871854	0.969987	2.666821
H	0.561476	1.573150	2.167074
H	–0.430560	–2.108331	–1.59692
H	0.949845	–1.274893	–1.85707
H	–0.436241	–0.771666	–2.53533
H	0.694988	–1.934506	1.623123
H	–0.753216	–1.615228	2.283895
H	–0.652098	–2.559568	0.966886
C	–0.198671	1.640633	–1.01017
O	–0.088694	2.574588	–1.67262
N	–2.405121	0.136561	–0.14218
H	–2.832793	1.007845	0.194566
H	–2.706043	0.045332	–1.12025
H	–2.861035	–0.626743	0.372531

Complex		$[Ru(CN)(NH_3)_4]^{+}$	
Atom	X	Y	Z
Ru	–0.228325	–0.029038	–0.002337
N	–0.379127	–1.599913	–1.674385
N	–0.255254	–1.524014	1.560180
N	0.019775	1.604851	–1.396516
H	–0.867996	–2.460063	–1.409307
H	0.547346	–1.909315	–1.986092
H	–0.848706	–1.277940	–2.525824
H	–0.285493	–1.013168	2.450587
H	–1.017190	–2.209424	1.588951
H	0.608722	–2.075536	1.591036
H	–0.048162	2.472716	–0.851908
H	–0.625627	1.699618	–2.187357

H	0.959205	1.618158	–1.807862
N	–2.259876	0.336957	0.202518
H	–2.709899	0.736334	–0.627550
H	–2.821593	–0.478929	0.466444
H	–2.359537	1.029708	0.958318
C	–0.022778	1.284715	1.407571
N	–0.021046	2.091315	2.265912

Compound		**NO^+**	
Atom	X	Y	Z
N	1.725484	–0.050451	–0.018854
O	2.795915	–0.082032	–0.042689

Compound		**NO**	
Atom	X	Y	Z
N	1.678268	–0.049059	–0.017802
O	2.837252	–0.083251	–0.043609

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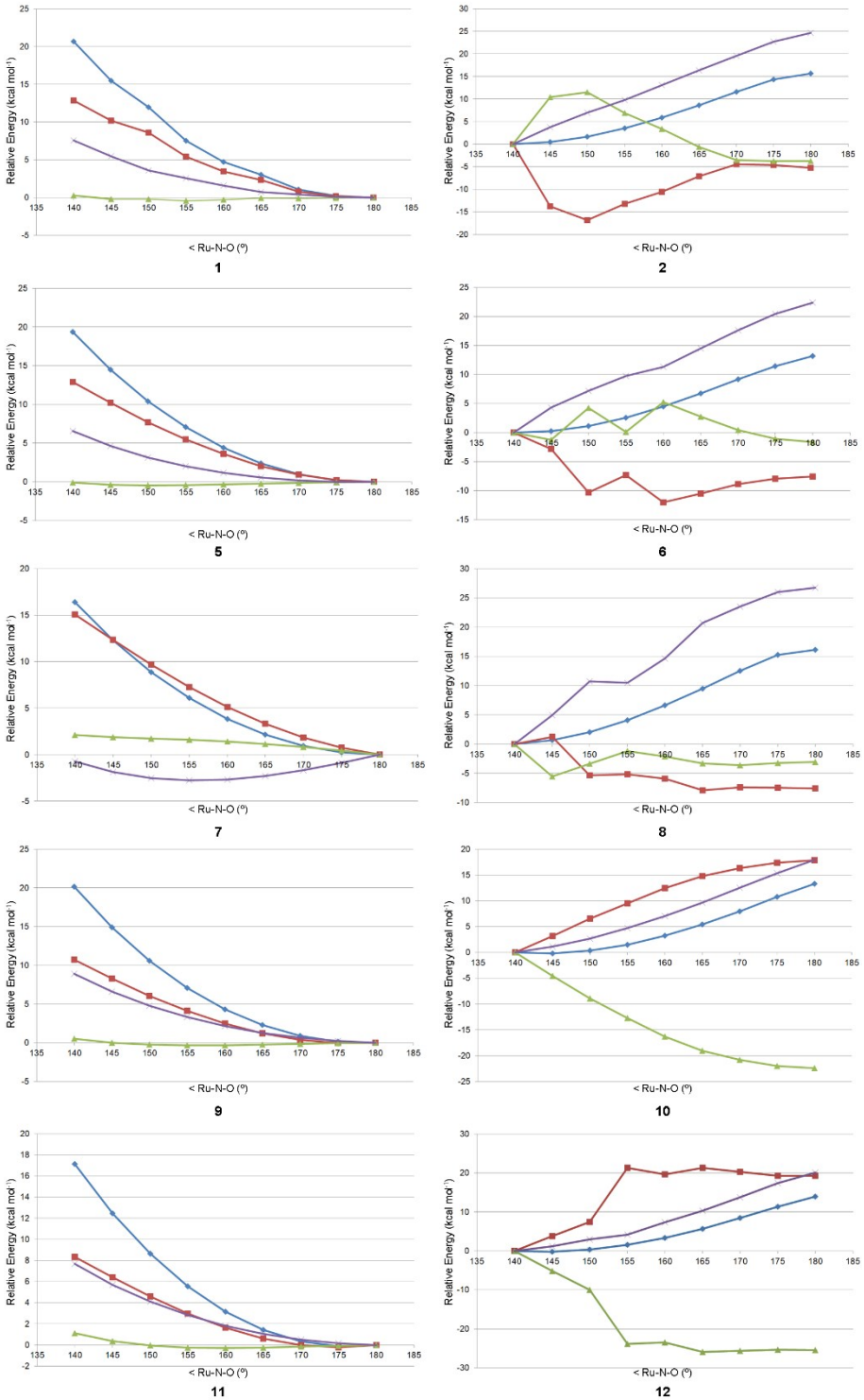

Figure S1. Relative values of the EDA components obtained by bending the Ru–N–O angles of **1**, **2** and **5**–**12**. Color code: $\Delta\Delta E_{int}$ (blue), $\Delta\Delta V_{elstat}$ (red), $\Delta\Delta E_{Pauli}$ (green) and $\Delta\Delta E_{oi}$ (purple).

Table S2. Relative values of the EDA components in the Ru–N–O angles (140–180°) of **1**–**8**.

		1					**3**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	20.68	12.85	0.26	7.57	140	17.63	6.20	0.69	10.74
145	15.46	10.19	–0.21	5.48	145	12.52	4.54	–0.14	8.12
150	11.99	8.60	–0.22	3.61	150	8.37	3.04	–0.63	5.97
155	7.54	5.43	–0.45	2.56	155	5.09	1.69	–0.80	4.21
160	4.71	3.44	–0.30	1.58	160	2.61	0.61	–0.78	2.80
165	3.01	2.32	–0.05	0.75	165	0.90	–0.08	–0.72	1.71
170	1.07	0.80	–0.12	0.39	170	–0.09	–0.49	–0.46	0.87
175	0.22	0.17	–0.05	0.10	175	–0.39	–0.47	–0.22	0.31
180	0.00	0.00	0.00	0.00	180	0.00	0.00	0.00	0.00
		2					**4**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	0.00	0.00	0.00	0.00	140	0.00	0.00	0.00	0.00
145	0.47	–13.73	10.42	3.78	145	0.42	–13.15	8.12	5.45
150	1.68	–16.82	11.54	6.96	150	1.58	–7.00	1.75	6.83
155	3.49	–13.24	6.91	9.81	155	3.37	–7.56	1.58	9.35
160	5.84	–10.55	3.34	13.05	160	5.61	–18.81	8.23	16.19
165	8.60	–7.14	–0.59	16.33	165	8.12	–17.22	5.26	20.08
170	11.56	–4.49	–3.49	19.54	170	10.70	–14.73	2.92	22.51
175	14.35	–4.64	–3.73	22.72	175	12.86	–15.25	2.13	25.98
180	15.63	–5.26	–3.73	24.62	180	13.59	–13.80	1.73	25.66
		5					**7**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	19.37	12.90	–0.08	6.55	140	16.39	15.05	2.08	–0.74
145	14.50	10.21	–0.36	4.65	145	12.29	12.33	1.85	–1.89
150	10.41	7.71	–0.45	3.15	150	8.87	9.69	1.72	–2.55
155	7.07	5.49	–0.43	2.00	155	6.07	7.27	1.59	–2.79
160	4.40	3.59	–0.34	1.16	160	3.82	5.11	1.40	–2.69
165	2.38	2.04	–0.23	0.56	165	2.12	3.30	1.12	–2.31
170	0.99	0.92	–0.12	0.19	170	0.91	1.82	0.79	–1.70
175	0.20	0.24	–0.05	0.01	175	0.21	0.72	0.41	–0.92
180	0.00	0.00	0.00	0.00	180	0.00	0.00	0.00	0.00
		6					**8**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	0.00	0.00	0.00	0.00	140	0.00	0.00	0.00	0.00
145	0.21	–2.83	–1.24	4.27	145	0.65	1.22	–5.55	4.97
150	1.10	–10.36	4.26	7.19	150	2.06	–5.32	–3.35	10.72
155	2.54	–7.33	0.13	9.73	155	4.09	–5.16	–1.22	10.46
160	4.46	–12.04	5.20	11.29	160	6.62	–5.93	–2.14	14.67
165	6.72	–10.52	2.72	14.50	165	9.50	–7.92	–3.33	20.74
170	9.14	–8.90	0.42	17.61	170	12.54	–7.38	–3.64	23.54
175	11.43	–7.93	–1.08	20.43	175	15.29	–7.47	–3.27	26.02
180	13.16	–7.55	–1.67	22.37	180	16.12	–7.59	–3.03	26.72

Table S3. Relative values of the EDA components in the Ru–N–O angles (140–180°) of **9**–**12**.

		9					**11**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	20.13	10.72	0.52	8.90	140	17.13	8.34	1.12	7.67
145	14.92	8.29	0.01	6.63	145	12.47	6.40	0.37	5.70
150	10.60	6.07	–0.24	4.78	150	8.63	4.58	–0.05	4.10
155	7.08	4.12	–0.34	3.31	155	5.55	2.98	–0.26	2.83
160	4.33	2.49	–0.31	2.16	160	3.15	1.62	–0.29	1.82
165	2.28	1.23	–0.23	1.29	165	1.43	0.62	–0.25	1.06
170	0.89	0.39	–0.14	0.66	170	0.33	–0.01	–0.17	0.51
175	0.13	–0.04	–0.06	0.23	175	–0.13	–0.22	–0.08	0.16
180	0.00	0.00	0.00	0.00	180	0.00	0.00	0.00	0.00
		10					**12**		
<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$	<	$\Delta\Delta E_{int}$	$\Delta\Delta V_{elstat}$	$\Delta\Delta E_{Pauli}$	$\Delta\Delta E_{oi}$
140	0.00	0.00	0.00	0.00	140	0.00	0.00	0.00	0.00
145	–0.20	3.20	–4.53	1.14	145	–0.22	3.75	–5.19	1.23
150	0.34	6.53	–8.89	2.71	150	0.33	7.44	–10.03	2.92
155	1.50	9.49	–12.70	4.71	155	1.55	21.29	–23.86	4.12
160	3.22	12.47	–16.28	7.03	160	3.36	19.58	–23.51	7.29
165	5.41	14.80	–19.04	9.66	165	5.70	21.29	–25.90	10.32
170	7.98	16.28	–20.80	12.51	170	8.42	20.24	–25.60	13.78
175	10.73	17.40	–22.03	15.36	175	11.33	19.29	–25.35	17.39
180	13.30	17.84	–22.42	17.90	180	13.90	19.23	–25.44	20.10

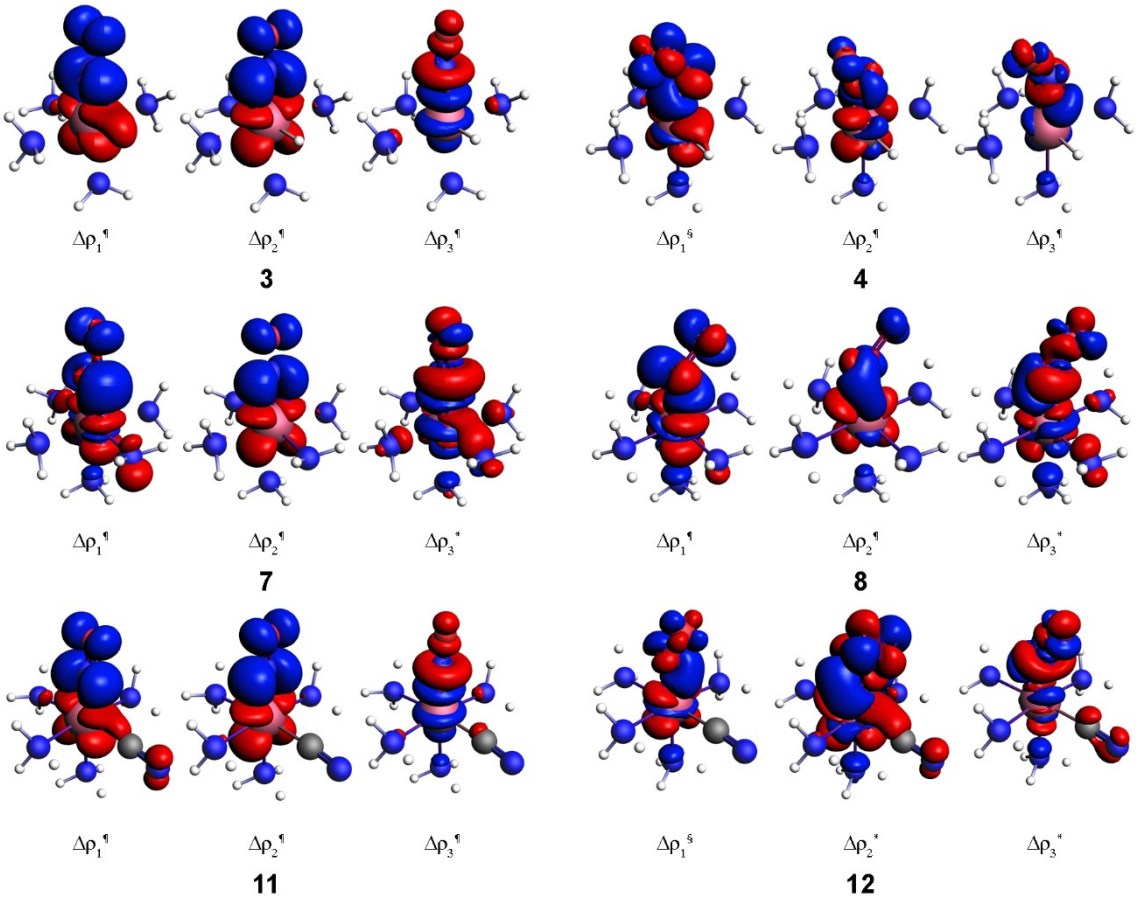

Figure S2. Selected density deformation channels, $\Delta\rho_{1-3}$, for the interacting fragments: i) $[RuL_{cis}(NH_3)_4]^{2+} - NO^+$ (**3**, **7** and **11**); and ii) $[RuL_{cis}(NH_3)_4]^{+} - NO^0$ (**4**, **8** and **12**). Red and blue regions indicate the electronic density outflow and inflow, respectively. Chosen contour values: *=0.001; ¶=0.003; §=0.005 a.u.

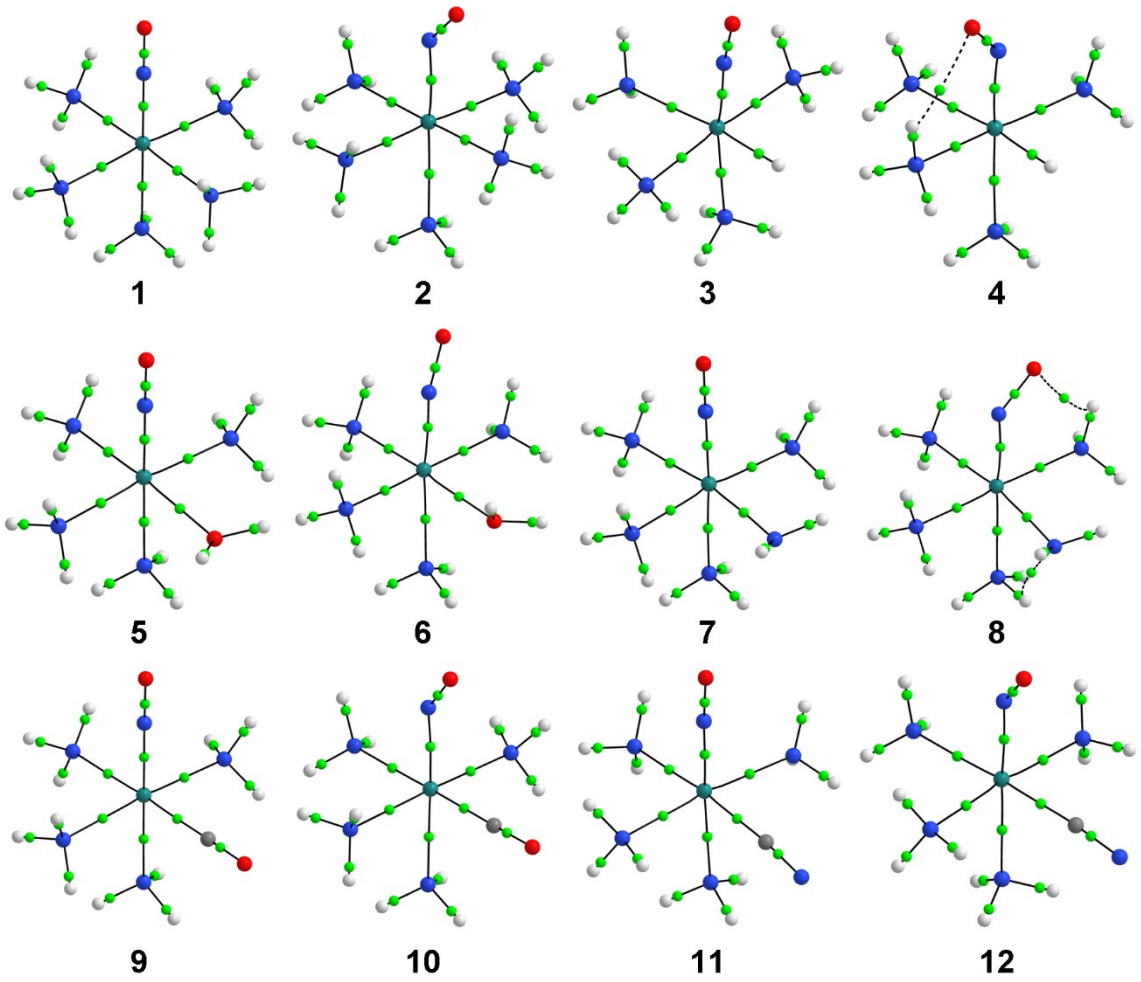

Figure S3. Topological map containing the bond paths (continuous or dashed lines connecting the cores) and bond critical points (small green points) for the structures studied in this paper. Atoms color code: H (white), C (gray), N (blue), O (red) and Ru (turquoise).

Table S4. Total energy density, H_b, and electron density, ρ_b, in the Ru–NO BCP of the compounds investigated. The values of all the parameters are in a.u.

Complex	H_b	ρ_b
1	–0.088	0.184
2	–0.081	0.174
3	–0.107	0.199
4[a]	–0.092	0.185
5	–0.084	0.180
6	–0.083	0.176
7	–0.106	0.199
8[b]	–0.096	0.188
9	–0.074	0.170
10	–0.061	0.153
11	–0.097	0.191
12	–0.082	0.175

[a] To compound **4**, there is one BCP related to N–H···O–N interaction with values of H_b and ρ_b equal to 0.003 and 0.015 a.u., respectively. [b] To compound **8**, there is one BCP related to N–H···O–N interaction with values of H_b and ρ_b equal to 0.003 and 0.016 a.u., respectively.