Supporting Information

For

Ruthenium Nitrosyls Derived from Tetradentate Ligands Containing Carboxamido-N and Phenolato-O Donors: Syntheses, Structures, Photolability and Time Dependent Density Functional Theory Studies

Nicole L. Fry, Michael J. Rose, David L. Rogow, Crystal Nyitray,

Manpreet Kaur, and Pradip K. Mascharak*

Department of Chemistry and Biochemistry, University of California,
Santa Cruz, CA 95064

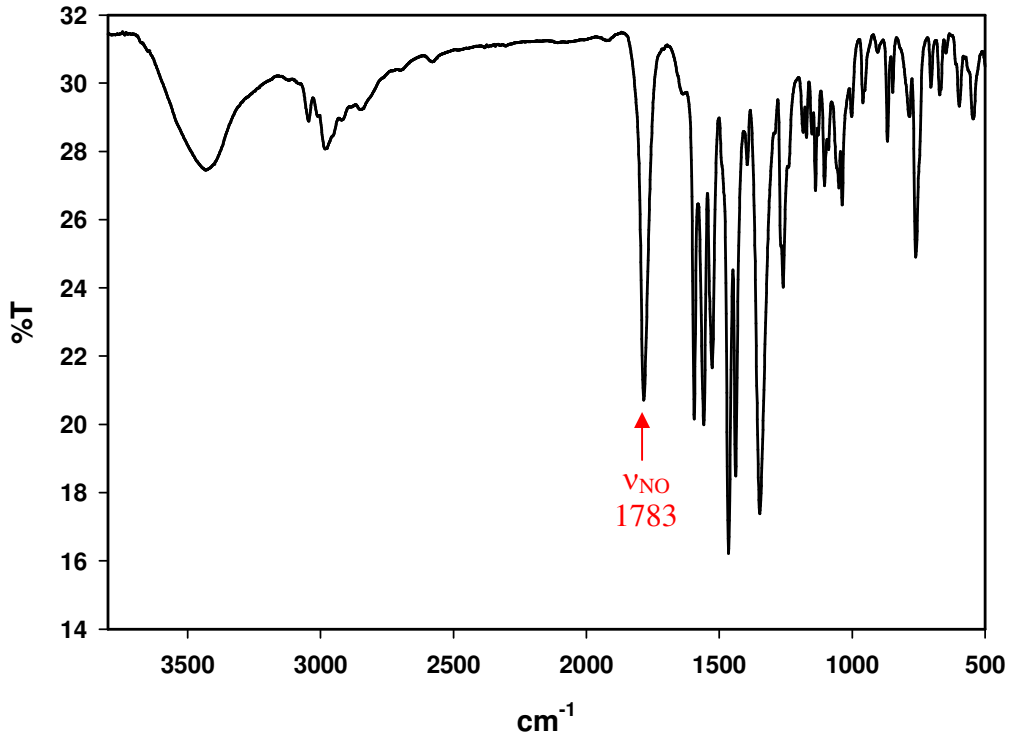

Figure S1. IR spectrum of **1** (in KBR disk)

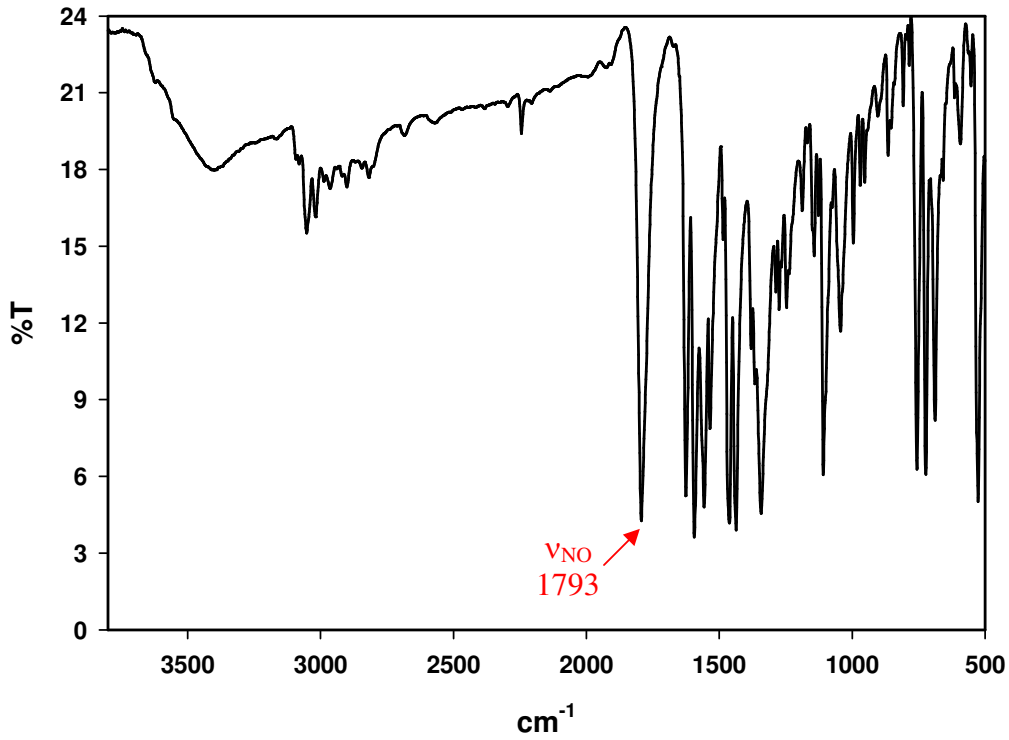

Figure S2. IR spectrum of **2** (in KBR disk)

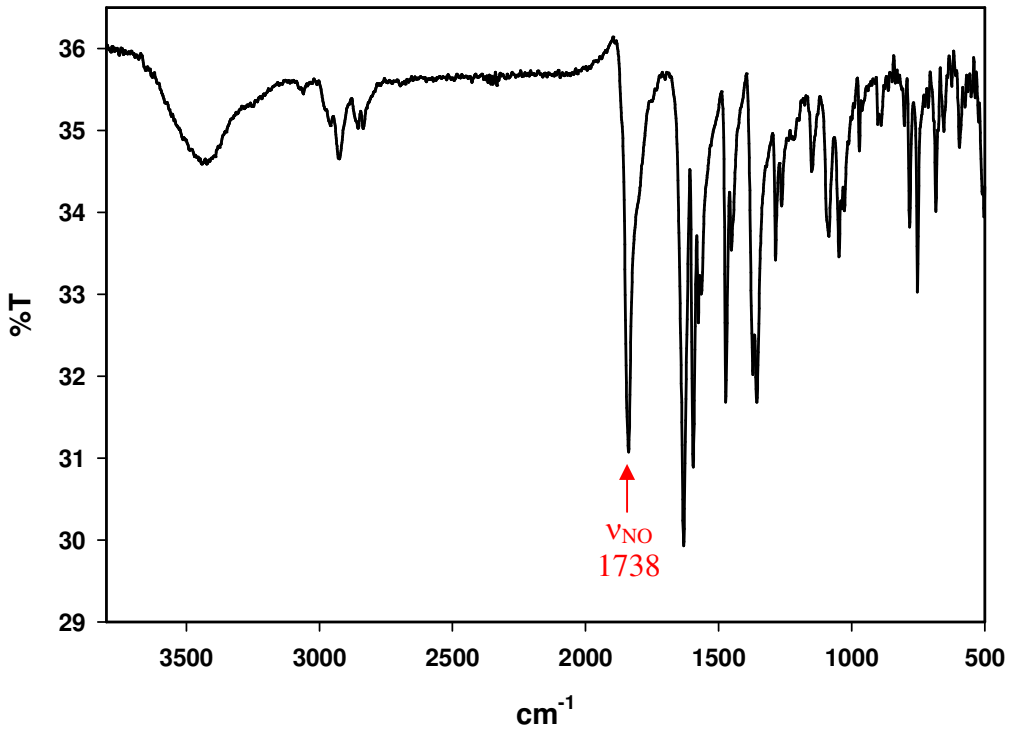

Figure S3. IR spectrum of **3** (in KBr disk)

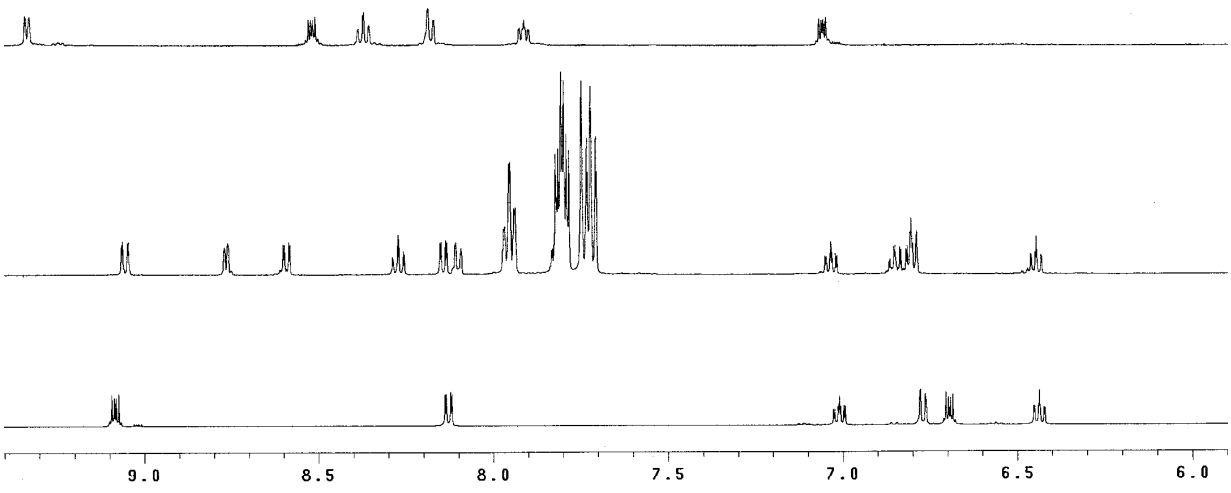

Figure S4. ^{1}H-NMR spectra (6-10 ppm) of **1**, **2**, and **3** in ($(CD_3)_2SO$) at 298 K

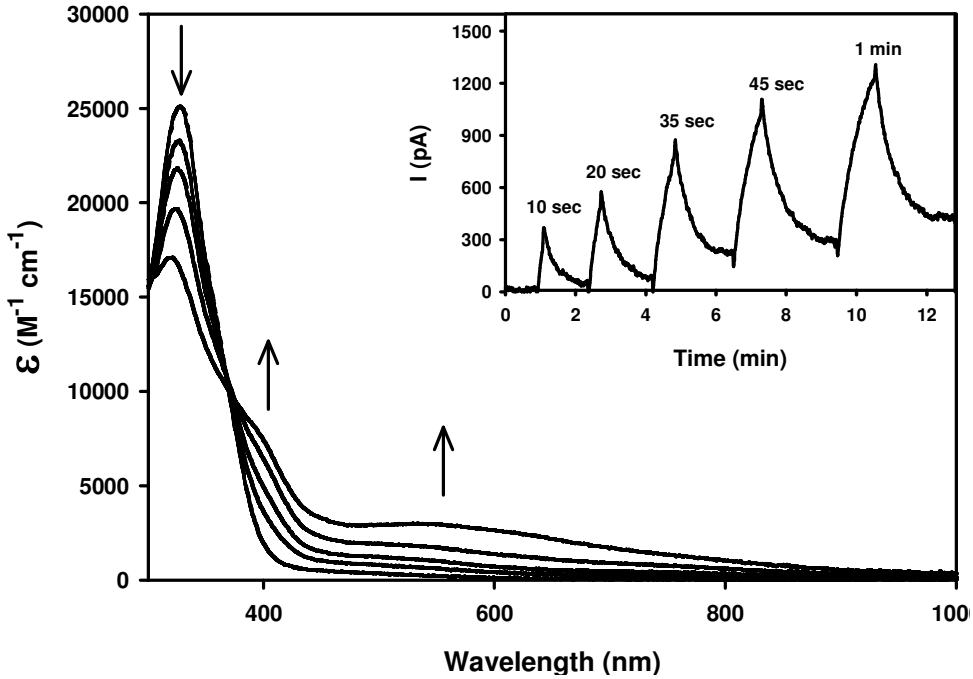

Figure S5. Changes in the electronic absorption spectrum upon photolysis of **1** in MeCN following illumination with UV light for 15 s intervals. Inset: NO amperogram of **1** in H_2O upon illumination with UV light for time periods as indicated.

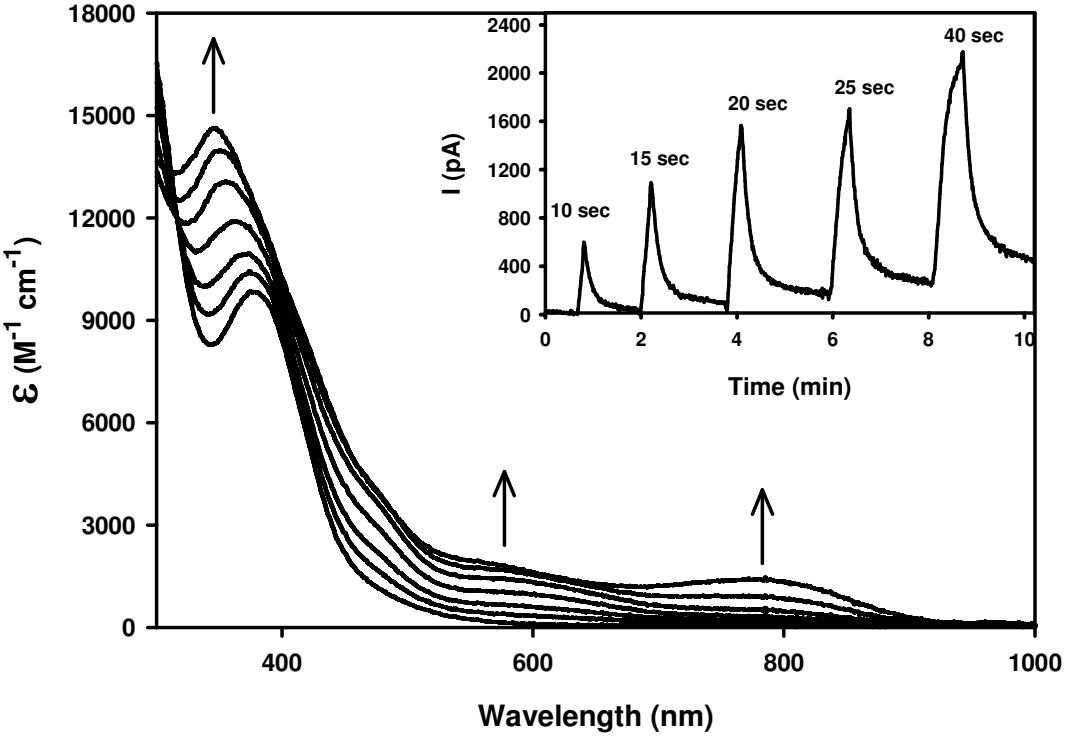

Figure S6. Changes in the electronic absorption spectrum upon photolysis of **3** in MeCN following illumination with UV light for 15 s intervals. Inset: NO amperogram of **3** in H_2O upon illumination with UV light for time periods as indicated.

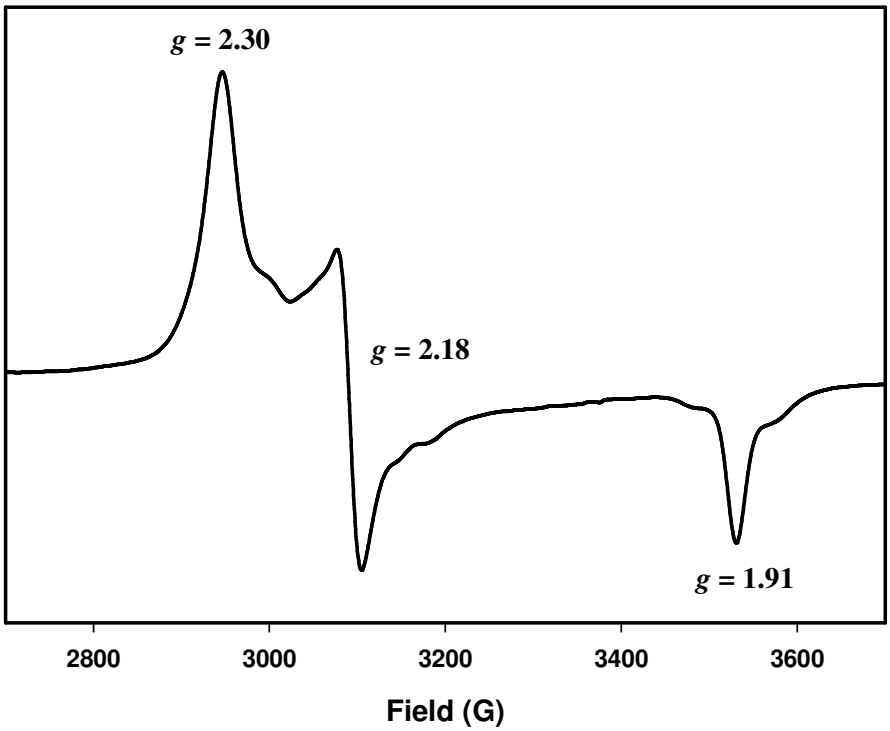

Figure S7. X-band EPR spectrum of the photoirradiated solutions of **3** in MeCN at 125 K. Spectrometer settings: microwave power, 50 mW; microwave frequency, 9.49 GHz; modulation frequency, 100 kHz; modulation amplitude, 2 G.

Table S1. DFT-optimized coordinates and gradient parameters for singlet excited state of **1**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
RU	44.0	9.7658859342	3.1768060394	2.6299117915
O	8.0	8.7641459945	2.7182037154	4.3472789586
O	8.0	10.8533515468	4.3788678639	3.8494380823
O	8.0	12.0954934049	5.0523129477	-0.3153116325
O	8.0	8.5719679685	4.7557481672	2.4766833035
O	8.0	11.5261128090	0.9007664406	2.5051462091
O	8.0	6.2991972423	1.6632748791	0.9565919436
N	7.0	8.4820290179	2.2338439309	1.3770433313
N	7.0	10.6202626414	3.7679741025	0.8772839160
N	7.0	10.8221477449	1.8183780336	2.6805795704
C	6.0	7.8144847340	1.8336116329	4.3297166295
C	6.0	10.0779929501	3.0744938112	-0.2195297233
C	6.0	8.9122549598	2.2904207770	0.0466952076
C	6.0	11.5982083128	4.7054778021	0.7726414184
C	6.0	7.0306233800	1.4495667964	3.1973738804
C	6.0	10.5996762104	3.0757936176	-1.5252838884
H	1.0	11.4739227256	3.6841980406	-1.7114158238
C	6.0	12.1159522328	5.3946952867	2.0194452593
C	6.0	11.6975289879	5.2425717722	3.3794104411
C	6.0	8.3273927955	1.5532735886	-0.9949132703
H	1.0	7.4355604900	0.9827810309	-0.7682575268
C	6.0	7.2379701210	1.8269837282	1.7521919266
C	6.0	12.2714543111	6.1146930326	4.3517717869
H	1.0	11.8749931564	6.0173831599	5.3600409159
C	6.0	13.7465648234	7.0989573166	2.7287447538
H	1.0	14.5587657358	7.7738192360	2.4690064565
C	6.0	10.0058725595	2.3273223743	-2.5386223072
H	1.0	10.4392573314	2.3515872903	-3.5378647119
C	6.0	5.9633855176	0.5623486021	3.4034267111
H	1.0	5.3597665144	0.3458581850	2.5246937427
C	6.0	13.1467153824	6.3131516774	1.7580159749
H	1.0	13.4498119958	6.3789135104	0.7163448794
C	6.0	7.5233273098	1.2084016159	5.5747365391
H	1.0	8.1648187165	1.4949001720	6.4051809772
C	6.0	8.8721715505	1.5646886829	-2.2754696909
H	1.0	8.4030132835	0.9736807570	-3.0609120184
C	6.0	5.6890614948	-0.0296872527	4.6274339109
H	1.0	4.8725563430	-0.7411229185	4.7268876558
C	6.0	6.5045831776	0.2898880395	5.7210377906
H	1.0	6.3490210409	-0.1848941587	6.6902185414
C	6.0	13.2736249231	7.0084466579	4.0452597206
H	1.0	13.6876357346	7.6406521369	4.8318945452
C	6.0	7.9692306969	5.1273891784	1.2849204858
H	1.0	7.2213411168	4.3829669111	0.9595730412
H	1.0	8.7105486763	5.2031056115	0.4720140613

C	6.0	7.2723446037	6.4757818861	1.4039108326
H	1.0	6.8227798956	6.7331405126	0.4322619853
H	1.0	7.9808131593	7.2655970944	1.6779777512
H	1.0	6.4761993249	6.4527084546	2.1572192550

E= -1557.5363983501 GMAX= 0.0031806 GRMS= 0.0007627

Ru	44.	1.6489837312E-03	-2.2468265573E-03	-1.4562290635E-04
O	8.	-8.3701610024E-06	3.6629738531E-04	5.9231582768E-05
O	8.	1.8285175193E-05	-4.1503803124E-04	3.4754207287E-04
O	8.	-2.2931678089E-04	1.3123235463E-04	9.8428016986E-06
O	8.	-3.1618823922E-04	1.8436215500E-04	1.4269513009E-04
O	8.	-2.5119264750E-03	3.1806111630E-03	-3.0286565036E-04
O	8.	1.1920805062E-03	1.6731362569E-03	1.2429281587E-03
N	7.	5.8457231546E-04	6.4631129014E-04	4.0628143446E-05
N	7.	-6.2150174633E-04	-2.5701592412E-04	2.2907397485E-05
N	7.	1.8067839042E-03	-2.5822716411E-03	-1.0369223845E-03
C	6.	-4.3709389270E-04	-1.0873134768E-04	-1.2188486913E-04
C	6.	-4.8261553489E-04	-2.1230322386E-04	4.2911011848E-04
C	6.	2.5475988986E-04	2.6181023181E-04	-2.9430418161E-04
C	6.	-3.6264259900E-04	-7.8223475038E-05	9.1872014756E-05
C	6.	2.5038733453E-04	8.6736010814E-04	2.9902011715E-04
C	6.	1.9697912760E-05	-2.0244790762E-04	-7.2491724721E-04
H	1.	5.7332711180E-04	3.5006214340E-04	2.6455552739E-04
C	6.	-3.3610595349E-04	1.7959760814E-05	5.3815056646E-04
C	6.	2.0629052457E-04	2.1680021328E-04	-4.1115204661E-04
C	6.	-5.5303655174E-04	-6.0883542931E-04	1.9820134164E-05
H	1.	-1.6367857831E-04	-4.9735622268E-04	4.5353573280E-04
C	6.	-2.2009588351E-03	3.5239935707E-04	-1.6951222097E-03
C	6.	-7.2752019641E-04	2.6984806110E-04	1.0708668775E-03
H	1.	-1.0129409817E-03	5.7049822216E-05	1.3079452398E-04
C	6.	4.1037578246E-04	-1.8630067003E-04	-6.5092219869E-04
H	1.	2.0243922538E-05	-1.2153428257E-03	2.9489625727E-04
C	6.	-2.2451567267E-04	-1.4805525342E-04	-2.3510120166E-04
H	1.	8.0134900844E-05	1.5845677510E-04	2.6906235703E-04
C	6.	-2.1466503887E-04	1.1074017599E-04	1.0687656144E-03
H	1.	-4.9069092879E-04	8.1732793409E-04	-6.2681199286E-04
C	6.	-1.1378558185E-04	3.4447436084E-05	7.5240665366E-04
H	1.	-3.8999391333E-04	-3.4129770937E-04	-5.4803094129E-04
C	6.	9.8097805296E-04	3.4889165359E-04	4.1322962506E-04
H	1.	7.2718781050E-04	5.3736233041E-04	-4.0586638372E-04
C	6.	1.8985626098E-04	-2.6695841761E-04	-9.4724956134E-04
H	1.	1.7079030941E-04	-1.0949713800E-04	4.7821835536E-04
C	6.	-5.7055516288E-05	4.0975466070E-06	-1.0775570319E-03
H	1.	6.7647726687E-04	3.3065962924E-04	-1.2467444906E-04
C	6.	7.0533557566E-04	-2.8458643118E-04	3.4027900326E-04
H	1.	1.3614111889E-03	-1.0629697542E-04	-2.4070627108E-04
C	6.	-4.2029648183E-04	-6.2851117823E-05	4.2163954482E-04
H	1.	-6.6164654352E-04	-1.5671392313E-04	3.0421884781E-04
C	6.	-2.5075642125E-04	1.0807374772E-03	9.0986736249E-04
H	1.	2.4944918698E-04	-4.1546949587E-04	5.4063785375E-04

H	1.	5.6279535642E-04	-5.1080832121E-04	7.7765510981E-04
C	6.	9.1956479427E-04	-9.3372661251E-04	9.7227208163E-04
H	1.	2.4606179076E-04	-9.5932857663E-04	-1.4295773588E-03
H	1.	-8.4330375809E-04	2.3742578923E-04	-6.6745885859E-04
H	1.	-2.2522422302E-04	6.7089617745E-04	-1.0199018216E-03

Table S2. DFT-optimized coordinates and gradient parameters for singlet excited state of **2**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
RU	44.0	10.5807725938	2.9357809547	2.5472612811
O	8.0	8.9894297216	6.6335021575	3.3372450269
O	8.0	9.6319898418	-0.1030960456	5.2084906789
O	8.0	12.0649865937	1.6500084746	2.0359507081
O	8.0	8.8000971826	2.1481212867	0.4028502011
O	8.0	11.8215931937	3.4907815531	3.9804750930
N	7.0	11.3645575720	4.6464138591	1.5548883222
N	7.0	9.3381584892	4.3286560745	3.2701273674
N	7.0	9.6464647880	1.7508508011	3.8722373810
N	7.0	9.5479341314	2.4646473570	1.2389255402
C	6.0	12.3734120369	4.7259718118	0.6906158882
H	1.0	12.8177307509	3.7748265408	0.4081447652
C	6.0	12.8201955483	5.9518905654	0.2080827247
H	1.0	13.6439481776	5.9866663786	-0.4984641311
C	6.0	12.1956043326	7.1130513673	0.6617343086
H	1.0	12.5355649627	8.0872777553	0.3214398501
C	6.0	11.1370469923	7.0148498422	1.5561117823
H	1.0	10.6008577039	7.8738232463	1.9481039507
C	6.0	10.7333245250	5.7545494781	1.9857874651
C	6.0	9.5742010110	5.6125268128	2.9541190585
C	6.0	8.4225101752	3.8136148505	4.1897978999
C	6.0	7.4210925937	4.5776332388	4.7950343407
H	1.0	7.3602772801	5.6276168466	4.5343380918
C	6.0	6.5537127638	3.9876622555	5.7083495810
H	1.0	5.7955158093	4.5946273522	6.1959345297
C	6.0	6.6699462643	2.6284134045	5.9887256162
H	1.0	5.9859285887	2.1551635885	6.6893952180
C	6.0	7.6620562938	1.8518565705	5.3927704530
H	1.0	7.7638965878	0.8008436045	5.6234181013
C	6.0	8.5796105130	2.4282999397	4.5001196897
C	6.0	10.0856753000	0.5088119595	4.2349907086
C	6.0	11.1348403975	-0.1702328214	3.3854471163
C	6.0	11.2252335982	-1.5531340935	3.6294317812
H	1.0	10.5405516419	-1.9472797643	4.3733895061
C	6.0	12.1265023594	-2.3824149802	2.9809126982
H	1.0	12.1383266377	-3.4493168365	3.1887335753
C	6.0	13.0167702427	-1.8156366166	2.0642503664

H	1.0	13.7534067355	-2.4307436740	1.5507632637
C	6.0	12.9646716859	-0.4612379074	1.8022324906
H	1.0	13.6454578710	0.0084120048	1.0941660675
C	6.0	12.0189987271	0.3974763393	2.4193865644
C	6.0	11.4372832858	3.7024988956	5.3035498515
H	1.0	10.7624223872	2.9048004969	5.6496694707
H	1.0	10.8781552040	4.6526668930	5.4065965400
C	6.0	12.6384293400	3.7355544800	6.2346088755
H	1.0	12.3253367228	4.0974108405	7.2234805621
H	1.0	13.4183459630	4.4025604659	5.8521228110
H	1.0	13.0716081617	2.7367667460	6.3566690176

E= -1499.0472550484 GMAX= 0.0031218 GRMS= 0.0007226

RU	44.	1.5962209983E-03	3.8694747904E-04	-2.0777793030E-04
O	8.	-6.3225401320E-04	4.7828515086E-04	5.6046370979E-04
O	8.	1.3734504886E-03	1.3525101286E-03	-8.6286631745E-04
O	8.	-8.6119855757E-05	-5.8124621176E-04	5.8154786777E-04
O	8.	1.7056003671E-04	-2.3498296789E-04	3.5193224658E-04
O	8.	-6.8069064544E-04	8.8116597912E-04	-4.7222862828E-04
N	7.	4.4275729569E-05	1.0385312982E-04	-5.4787189539E-04
N	7	-1.8089951593E-04	-4.7465839601E-04	1.2557946650E-04
N	7.	4.7581326048E-04	3.7854824598E-04	1.1370758278E-04
N	7.	-8.1936955483E-04	-4.2285412610E-04	-3.3414635984E-05
C	6.	-5.6316403705E-04	-4.2864308956E-04	-1.5164088599E-04
H	1.	-5.3929882213E-04	-7.5263198278E-04	-4.3942568142E-04
C	6.	3.2245982441E-04	-3.5720590694E-05	-5.9902323540E-04
H	1.	4.4313842856E-05	-3.0696776228E-04	-4.3069037793E-04
C	6.	-4.0706562474E-04	9.8945576001E-04	3.8243923727E-04
H	1.	2.1593775519E-05	-3.4115216993E-04	6.0437495790E-04
C	6.	7.6268610434E-04	2.9012202490E-04	-5.9037227571E-04
H	1.	-4.4000717933E-04	4.8786831561E-04	4.6168043222E-04
C	6.	-1.6833495590E-04	-2.0539208949E-04	8.0100654045E-05
C	6.	8.7513362584E-04	-7.8885181873E-04	-6.0519269064E-04
C	6.	2.1745548412E-04	-9.6622747858E-04	2.7482120337E-04
C	6.	-5.2075135243E-05	9.3561275148E-04	-2.3990738020E-04
H	1.	2.1498690305E-04	4.4279361074E-05	-1.0000108895E-03
C	6.	-3.0878761883E-04	6.9203828313E-04	7.3459653058E-04
H	1.	1.1472914550E-03	2.8818204653E-04	2.3902836688E-05
C	6.	-2.8822533485E-04	-1.3581330867E-04	5.1501534148E-04
H	1.	3.4660684443E-04	9.9857546617E-05	-2.5973316398E-04
C	6.	-1.2688364860E-04	-1.2247407696E-03	9.4588084241E-05
H	1.	-4.2303466544E-04	-4.7014204240E-04	-7.4752820475E-04
C	6.	-3.0058951393E-04	7.4814917644E-04	3.1118819081E-04
C	6.	-4.4004486111E-04	-1.1575791425E-03	2.3002626210E-03
C	6.	8.8520576070E-04	9.6320591057E-04	-7.6236298625E-04
C	6.	-1.6593737331E-03	-6.5303829912E-04	1.5480294494E-03
H	1.	1.3000709520E-06	3.8646773332E-04	-2.2115926691E-04
C	6.	1.2040426262E-03	-1.8934976088E-04	-1.5581634174E-03
H	1.	-4.9102393215E-04	9.0904865472E-05	-2.1827563870E-04
C	6.	-1.9617556134E-04	-1.4803527855E-03	3.3414418035E-04

H	1.	-8.4447821004E-05	8.0179332975E-04	7.7874808717E-05
C	6.	-3.7992413363E-04	8.0964588659E-04	2.0024702440E-04
H	1.	5.4054815425E-04	1.0481468417E-03	-4.5729559759E-04
C	6.	1.4983203855E-04	2.0176852782E-04	1.0069227220E-04
C	6.	3.1218387235E-03	-2.3797854796E-04	-2.0905201545E-05
H	1.	-3.9802517246E-04	-1.4167429014E-03	-1.0264937939E-03
H	1.	-1.1611299126E-03	4.1416821260E-04	2.3320828294E-04
C	6.	-1.1922733261E-03	7.5924778930E-05	-5.2758879080E-04
H	1.	-8.2841178820E-04	6.5266145677E-04	-4.2455053551E-05
H	1.	5.5528926351E-05	-1.0455795468E-03	6.4222385382E-04
H	1.	-7.2351431091E-04	-5.0917134219E-05	1.3697631046E-03

Table S3. DFT-optimized coordinates and gradient parameters for singlet excited state of **3**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	**CHARGE**	**X**	**Y**	**Z**
RU	44.0	7.5730481687	3.2464254468	6.2007559265
O	8.0	5.8657620035	-0.3329862850	5.1990574939
N	7.0	8.7897590545	3.2689705401	4.9540321192
N	7.0	6.4219556519	1.9217401193	5.2723040552
O	8.0	9.5544049843	3.2805009518	4.0834908754
C	6.0	3.7390020110	2.5656039216	2.7615082233
H	1.0	3.0573783246	2.0228998960	2.1112672557
N	7.0	8.3256834237	1.4450986799	7.0861085829
C	6.0	7.6230132375	0.3894631974	6.6301445882
C	6.0	9.6124384719	0.0024134970	8.4770888353
H	1.0	10.4111526817	-0.1067258443	9.2018897664
C	6.0	7.8809240252	-0.8977586158	7.0839792170
H	1.0	7.2773343812	-1.7040976931	6.6837115286
C	6.0	6.5267234151	0.6202725077	5.6055713908
C	6.0	9.2922865930	1.2609900508	7.9870882385
H	1.0	9.8223060716	2.1485517052	8.3201509782
C	6.0	8.8908908642	-1.0948443446	8.0182457349
H	1.0	9.1161616108	-2.0919005525	8.3846438508
O	8.0	6.3264129887	3.1636574186	7.7053056310
C	6.0	5.4936647505	2.5428013715	4.4176832680
C	6.0	4.6052992597	1.8557110756	3.5875608438
H	1.0	4.6085743538	0.7723553550	3.6044472841
C	6.0	4.9499821626	3.4687932226	7.7082715460
C	6.0	4.0627150682	2.2213137134	7.7129229728
O	8.0	5.8838182864	6.8445956852	5.1877083722
N	7.0	6.4016574644	4.5813811040	5.3081331250
C	6.0	3.7431639219	3.9577244811	2.7617444768
H	1.0	3.0660420991	4.5047705891	2.1104059242
N	7.0	8.3148951235	5.0659010314	7.1117915444
C	6.0	7.6145558914	6.1211729655	6.6496869347
C	6.0	9.6145093661	6.5221510752	8.4808712147

H	1.0	10.4186345659	6.6364308731	9.1990114833
C	6.0	7.8781678652	7.4129797164	7.0895628273
H	1.0	7.2789510239	8.2188841939	6.6815529224
C	6.0	6.5224416114	5.8876967291	5.6205159501
C	6.0	9.2901638549	5.2599397632	8.0019064441
H	1.0	9.8276189779	4.3765854455	8.3341433188
C	6.0	8.8909597814	7.6168802415	8.0193372466
H	1.0	9.1181569576	8.6164436190	8.3782873611
C	6.0	5.4922629449	3.9686347422	4.4238375948
C	6.0	4.6099122666	4.6620229111	3.5923223569
H	1.0	4.6164987260	5.7453387106	3.6110298944
H	1.0	4.7620210740	4.0667620012	8.6131125260
H	1.0	4.5201429718	1.4511447281	7.0869801018
H	1.0	3.0644206130	2.4283164939	7.3021539734
H	1.0	4.6867637933	4.0966774040	6.8477114917
H	1.0	3.9366702617	1.8131290606	8.7221913590

E= -1440.4473854523 GMAX= 0.0021487 GRMS= 0.0007092

RU	44.	-6.2534186981E-04	-3.6372492342E-05	-5.3382824726E-04
O	8.	3.3941185170E-04	1.3694965358E-04	3.2424610934E-04
N	7.	7.7754012372E-04	1.0216546737E-04	-2.5029265827E-04
N	7.	3.2181159326E-04	-1.7191838677E-03	8.0479806605E-04
O	8.	-1.2615577972E-03	-4.1900606413E-04	5.4319572063E-05
C	6.	4.7010470581E-04	-2.7589987104E-04	3.6465564826E-04
H	1.	-2.5922946014E-04	2.4259639438E-06	-4.5859658747E-04
N	7.	-5.2641179346E-04	-4.0160880253E-04	-3.9000391106E-04
C	6.	1.1074748657E-03	-2.6840030568E-04	1.0702598707E-03
C	6.	-2.2366253864E-04	-1.3209713036E-04	-3.1019821330E-04
H	1.	-3.0898424145E-04	8.6444142181E-05	-6.1639307440E-04
C	6.	-7.6006075844E-04	2.5926527744E-04	-6.4130677702E-04
H	1.	4.3546117425E-04	4.0975004128E-04	3.1300657018E-04
C	6.	-8.4367522548E-04	-6.6919928261E-04	-5.9066910245E-04
C	6.	4.6646798896E-04	6.7588835279E-04	3.1266761647E-04
H	1.	7.8829411426E-04	5.2581886742E-04	5.0974896090E-04
C	6.	9.6141713891E-04	3.5592764960E-04	8.8471998420E-04
H	1.	1.3263321335E-04	3.0522728938E-04	-5.1042652907E-05
O	8.	6.9460502815E-04	-2.1204179773E-03	-3.9934953910E-04
C	6.	-8.3279355514E-04	5.9188548386E-04	-1.0492031809E-04
C	6.	3.5664167484E-05	1.1040957913E-03	3.4918938690E-04
H	1.	-2.3936962573E-04	-2.8299287805E-04	-1.7095709887E-04
C	6.	-2.0908397609E-03	4.7173039559E-04	4.8700126697E-05
C	6.	-7.9981686106E-04	3.4565360525E-04	-3.0862943116E-04
O	8.	7.7535019954E-05	4.0357272388E-04	-1.0107607164E-04
N	7.	2.1148627384E-04	1.9766327377E-03	1.0647431169E-03
C	6.	4.9501445301E-04	3.4425590088E-04	4.2088584801E-04
H	1.	-2.7816965136E-04	-8.7476087700E-08	-4.7532712756E-04
N	7.	-6.5524320071E-04	4.6209456324E-04	-3.6306926612E-04
C	6.	1.1595485527E-03	5.7364506634E-04	1.0374559293E-03
C	6.	-1.5818707755E-04	2.2852630808E-04	-3.8320907031E-04
H	1.	-3.2736697697E-04	7.5303432023E-06	-5.4573578719E-04

C	6.	-6.4617565812E-04	-1.2683132296E-04	-7.3078417365E-04
H	1.	5.7591202736E-04	-1.2731193832E-04	3.5856777939E-04
C	6.	-4.5423824244E-04	3.9392488406E-05	-4.0513654047E-04
C	6.	5.5311172623E-04	-4.7171038466E-04	1.8980733514E-04
H	1.	9.3708138468E-04	-3.6107231482E-04	2.4229416943E-04
C	6.	9.3966764755E-04	-1.3364747491E-04	9.1717475418E-04
H	1.	1.0928142303E-04	-1.8247463897E-04	1.2432707770E-04
C	6.	-8.1262903836E-04	-5.2990641751E-04	-1.2089151559E-04
C	6.	1.1767348889E-05	-1.0096436154E-03	2.8491049596E-04
H	1.	-2.2395855184E-04	3.4112685314E-04	-4.0939575064E-04
H	1.	1.5843756940E-03	-4.3822306267E-04	6.0764742111E-04
H	1.	2.1486667268E-03	8.2294818843E-04	3.5304468833E-04
H	1.	-1.8394179855E-03	-1.5875729832E-03	-1.9239538328E-03
H	1.	3.3134804162E-04	3.8843102086E-05	-6.9313280927E-04
H	1.	-1.4985524150E-03	6.8186404490E-04	3.4072902937E-04

Table S4. Calculated (TD-DFT) energies (E, nm), oscillator strengths (*f*), and nature of transitions [a] in the complexes **1** , **2**, and **3** (in the range of $E \geq 300$ nm, only transitions with $f > 0.011$ are given)

[(hypbe)Ru(NO)(OEt)]$^{2-}$ (1)

Energy (nm)	Oscillator Strength (*f*)	Transition
335	0.2054	π(PDA)-*p*(OEt) → π*(RuNO)- *p*(OEt)
315	0.0487	π(PDA) → π(L)
309	0.1378	π(PhO)-σ(OEt)-π(RuNO) → π*(RuNO)- *p*(OEt)
306	0.0948	π(PhO)-σ(Nca) → π(L)
300	0.0567	π(PhO)-σ(Nca) → π*(RuNO)-σ(OEt)

[(hypyb)Ru(NO)(OEt)]$^{1-}$ (2)

Energy (nm)	Oscillator Strength (*f*)	Transition
420	0.0377	π(PDA)-π(PhO)-π(RuNO) → π*(RuNO)-π*(Npy)
387	0.0257	π(PhO)-π(RuNO)-π(PDA) → π*(RuNO)-π*(Npy)
335	0.0462	π(PDA)-*p*(OEt) → π*(RuNO)-π(Npy)
312	0.0521	π(PDA)-*p*(OEt) → π*(RuNO)-π*(Npy)
303	0.0923	π(PhO)-dπ(xy) → π*(RuNO)-π(Npy)
300	0.1004	π(PDA)-π(PhO)-π(RuNO) → π(L)-π*(RuNO)-π(Npy)

[(bpb)Ru(NO)(OEt)] (3)

Energy (nm)	Oscillator Strength (*f*)	Transition
390	0.0761	π(PDA)-π(RuNO) → π*(Npy)-π*(RuNO)
389	0.0404	π(PDA)-π(RuNO) → π(Npy)
313	0.0266	π(PDA)-π(RuNO) → π(L)
307	0.0284	π(PDA)-π(RuNO) → d(x^2-y^2)-π(Npy)
306	0.0368	dπ(xy)-σ(OEt) → π(Npy)
300	0.0335	π(PDA)-*p*(OEt)→ π(Npy)

[a] Orbitals with greater contributions are listed first.

Table S5. DFT-optimized coordinates and gradient parameters for lowest excited triplet state of **1**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
RU	44.0	9.7115922200	3.2502277731	2.6253312454
O	8.0	8.8037096830	2.6588974574	4.3387337740
O	8.0	10.8500836123	4.4198908201	3.8457962489
O	8.0	12.0921492908	5.0229723991	-0.3017399457
O	8.0	8.5215514405	4.8061927908	2.4746154669
O	8.0	11.5803852292	1.0181834660	2.3176977953
O	8.0	6.3070685103	1.5914175679	0.9471951984
N	7.0	8.4693031218	2.2467064640	1.3723215961
N	7.0	10.6565385235	3.7097202812	0.9227538022
N	7.0	10.7360411520	1.6263008203	2.8746251121
C	6.0	7.8341610436	1.7917234749	4.3238463954
C	6.0	10.1087384585	3.0361430991	-0.1974625276
C	6.0	8.9196019974	2.2771775705	0.0548295417
C	6.0	11.6185774468	4.6827126045	0.7961286211
C	6.0	7.0405850105	1.4210059979	3.1919612933
C	6.0	10.6235059528	3.0531223089	-1.5040608411
H	1.0	11.4929718445	3.6596246361	-1.7003705353
C	6.0	12.1363445684	5.3977289272	2.0201794192
C	6.0	11.7119150953	5.2609185966	3.3844433199
C	6.0	8.3274828753	1.5601922563	-0.9963024167
H	1.0	7.4204400855	1.0087128795	-0.7838870318
C	6.0	7.2432153864	1.7951192649	1.7431395749
C	6.0	12.3070264820	6.1281051354	4.3512658646
H	1.0	11.9291444686	6.0323707857	5.3665290602
C	6.0	13.7545511172	7.1221628592	2.7111061726
H	1.0	14.5521659916	7.8136603104	2.4439462042
C	6.0	10.0164389197	2.3281172894	-2.5298582751
H	1.0	10.4420617820	2.3640077506	-3.5314820059
C	6.0	5.9670708866	0.5448942109	3.3992100846
H	1.0	5.3673904054	0.3235078416	2.5212530248
C	6.0	13.1591462997	6.3232364290	1.7475873758
H	1.0	13.4713651613	6.3910509445	0.7086499096
C	6.0	7.5219279725	1.1873900832	5.5731203681
H	1.0	8.1572624290	1.4732205766	6.4087749330
C	6.0	8.8765760233	1.5743576336	-2.2745059686
H	1.0	8.4033509105	0.9929711112	-3.0661376368
C	6.0	5.6752566453	-0.0313252147	4.6294854886
H	1.0	4.8517311044	-0.7363660120	4.7252244232
C	6.0	6.4812179157	0.2928244574	5.7248024858
H	1.0	6.2966193117	-0.1575220117	6.7018530811
C	6.0	13.3011884284	7.0245695816	4.0317072252
H	1.0	13.7303231934	7.6530336699	4.8145527485

C	6.0	7.9294551016	5.1490009911	1.2658771805
H	1.0	7.1918892632	4.3990960064	0.9398205034
H	1.0	8.6831556120	5.2168997292	0.4636958888
C	6.0	7.2422492943	6.5023491473	1.3982686529
H	1.0	6.7839296795	6.7907230054	0.4418365487
H	1.0	7.9710730143	7.2689618655	1.6876829212
H	1.0	6.4622906187	6.4637321367	2.1683822245

E= -1557.4997374986 GMAX= 0.0023164 GRMS= 0.0007795

RU	44.	-3.4513368429E-04	1.6923187324E-05	-5.6118778981E-04
O	8.	1.2533996983E-03	7.1277071123E-04	3.7640923726E-04
O	8.	-2.1815780706E-04	3.1480715948E-05	4.8058674365E-04
O	8.	-6.4693977722E-04	5.1259837004E-04	6.3676347125E-06
O	8.	-2.6617770322E-04	6.7087133741E-04	1.2968232120E-04
O	8.	-2.2765853046E-03	9.8594757485E-04	2.0269201806E-03
O	8.	-8.5653506851E-04	1.1804061116E-03	-6.0959560031E-04
N	7.	1.3278373740E-03	1.4480629828E-04	-1.2225169660E-03
N	7.	-1.7096874698E-04	-7.6834798000E-04	4.5757308526E-04
N	7.	3.4747703233E-04	-1.8274142309E-03	-1.9743313679E-03
C	6.	-1.0205859888E-03	-1.1193457874E-03	-4.4228870206E-04
C	6.	7.3148977509E-04	-4.2432524116E-04	-7.7507571983E-04
C	6.	-6.0038808229E-04	-8.8515343971E-04	9.6868654270E-04
C	6.	-1.2829663707E-04	-3.0309602065E-05	1.5504934636E-04
C	6.	7.6103564916E-06	3.1773397780E-05	6.3863247312E-04
C	6.	1.4707714709E-03	1.4123388559E-03	2.5324253620E-04
H	1.	-1.4149788988E-03	-1.2641882374E-04	-5.9613415194E-04
C	6.	1.0290062065E-03	5.8762070870E-04	-9.5986927838E-04
C	6.	-3.3578813594E-04	-1.0989215734E-05	5.2285751855E-04
C	6.	2.6133270145E-04	1.0183662519E-04	1.0379052548E-03
H	1.	-4.2946333768E-04	-5.0680197724E-04	-1.3150851079E-04
C	6.	-1.8350011429E-04	3.1579055706E-04	1.0070103941E-03
C	6.	-9.6092775885E-04	-1.4795866884E-04	3.9233798035E-04
H	1.	-4.6397740696E-04	3.5340140715E-04	9.8337061073E-05
C	6.	-8.2125223506E-04	-2.0137100801E-04	2.0854680309E-03
H	1.	4.1020748806E-04	-1.0777182219E-05	4.4979389476E-04
C	6.	-2.1120533355E-04	2.4564036687E-04	-8.3564995058E-04
H	1.	-5.4648951308E-04	-9.2228792299E-05	3.2435629701E-04
C	6.	6.8659198308E-04	1.3798029270E-03	-1.7528569017E-03
H	1.	1.2523983998E-05	6.9276748204E-04	3.8277886284E-04
C	6.	-1.0492045804E-03	-1.0121687939E-03	7.7022396812E-04
H	1.	7.5466532922E-04	3.5698449058E-04	-2.8807656188E-04
C	6.	1.0638959346E-03	5.0157832986E-04	-9.2146865468E-05
H	1.	5.7677895178E-04	2.9113584733E-04	6.5598002955E-05
C	6.	-2.9153089961E-04	-1.4265380317E-04	-4.4473548039E-04
H	1.	1.1067037826E-04	-6.7700914641E-04	8.6568310894E-05
C	6.	5.6031590621E-04	-1.2086138754E-04	1.9046013239E-03
H	1.	4.8127295664E-04	-2.6713787983E-04	-3.9893685592E-04
C	6.	-1.0977503730E-04	5.0996103320E-05	-1.4597171244E-03
H	1.	4.3097284009E-04	-3.4843262547E-04	3.9530035441E-04
C	6.	6.8678017407E-05	-1.2632604681E-04	-2.3164040423E-03

H	1.	-6.6211617800E-06	-6.0060302925E-05	6.0838988431E-04
C	6.	2.8864200774E-04	-2.0404342375E-03	-1.1788428398E-03
H	1.	1.0462579673E-03	7.2255516150E-04	4.4174795915E-04
H	1.	-4.6323266114E-04	1.1361340505E-04	6.3133397388E-04
C	6.	4.1299808061E-05	3.5732310626E-04	-2.7805957164E-04
H	1.	4.9567154911E-04	-7.5883153162E-04	-4.3812446150E-04
H	1.	3.7463766507E-04	1.0007829943E-04	4.4957781955E-06
H	1.	-1.4291507312E-05	-1.6568367322E-04	5.3803791330E-05

Table S6. DFT-optimized coordinates and gradient parameters for lowest excited triplet state of **2**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
RU	44.0	10.6290282425	2.9544937327	2.5881087384
O	8.0	8.9758725664	6.5996098741	3.3338629446
O	8.0	9.5918783193	-0.1173563537	5.1798992059
O	8.0	12.0308846788	1.6420637373	1.9944921457
O	8.0	8.6297980981	2.3166790544	0.5405863283
O	8.0	11.8672455234	3.4953856848	4.0310191117
N	7.0	11.3872953473	4.6457451193	1.5799895222
N	7.0	9.3080094244	4.2895671925	3.2085610902
N	7.0	9.6206786254	1.7490997136	3.8499349276
N	7.0	9.6988137753	2.2850222014	1.0261857922
C	6.0	12.3984943143	4.7296199566	0.7166363805
H	1.0	12.8615369501	3.7851816794	0.4403818241
C	6.0	12.8248738014	5.9574228069	0.2205209472
H	1.0	13.6445112963	5.9929085423	-0.4886591349
C	6.0	12.1905449874	7.1151296473	0.6610074030
H	1.0	12.5156431609	8.0885156547	0.3011809979
C	6.0	11.1289290004	7.0175752996	1.5523924280
H	1.0	10.5922520269	7.8828134842	1.9312710997
C	6.0	10.7340412092	5.7548645667	1.9813724183
C	6.0	9.5594970640	5.5935719819	2.9241145157
C	6.0	8.3998635088	3.8036592745	4.1563078652
C	6.0	7.4112168917	4.5743928563	4.7797591541
H	1.0	7.3403501950	5.6282302892	4.5360588587
C	6.0	6.5466804212	3.9865795802	5.6984297280
H	1.0	5.7741645962	4.5857626997	6.1719895293
C	6.0	6.6715956740	2.6318716572	5.9928974198
H	1.0	5.9825921545	2.1585401607	6.6874581033
C	6.0	7.6715965553	1.8561683612	5.4108738682
H	1.0	7.7873447477	0.8138864111	5.6689117313
C	6.0	8.5679779921	2.4220487826	4.4874446312
C	6.0	10.0498433803	0.5048548694	4.2108697728
C	6.0	11.1115333431	-0.1749597600	3.3689333343
C	6.0	11.2254068635	-1.5488743966	3.6324715958
H	1.0	10.5549316101	-1.9497035105	4.3896560737

C	6.0	12.1350357543	-2.3773612017	2.9939035169
H	1.0	12.1586125984	-3.4404738466	3.2127512059
C	6.0	13.0130469374	-1.8131204178	2.0641048166
H	1.0	13.7550731660	-2.4288548434	1.5588827695
C	6.0	12.9418176970	-0.4651993157	1.7802574798
H	1.0	13.6158680174	0.0022946768	1.0654335420
C	6.0	11.9897679763	0.3898308104	2.3901322411
C	6.0	11.4608214711	3.7068876301	5.3427855055
H	1.0	10.7712549789	2.9271965055	5.7031193356
H	1.0	10.9137194578	4.6670301703	5.4235326165
C	6.0	12.6694032262	3.7431108555	6.2642516757
H	1.0	12.3571995150	4.0750951431	7.2619141521
H	1.0	13.4255931245	4.4368872206	5.8807209330
H	1.0	13.1222930142	2.7501001114	6.3457019076

E= -1499.0107127056 GMAX= 0.0059525 GRMS= 0.0010372

RU	44.	1.5203155006E-04	-1.0796057006E-04	-7.9632399182E-04
O	8.	-1.9539966606E-04	1.7126226516E-04	1.2590475387E-03
O	8.	-6.7758054192E-04	8.0844206418E-05	2.6033680594E-03
O	8.	7.6414711425E-04	3.0967255631E-04	-6.0106350706E-04
O	8.	5.9525384451E-03	-1.1511203479E-03	1.0268125108E-03
O	8.	-9.8777964307E-05	4.7821259318E-04	1.7866973825E-03
N	7.	-4.9810764535E-04	2.0506311189E-04	-1.7740750985E-04
N	7.	-1.7965061533E-03	-9.2529737614E-04	1.1204915520E-03
N	7.	-2.1910680810E-03	9.2034082794E-04	-1.2362277669E-04
N	7.	-2.0599840571E-03	-1.6658194912E-03	-1.6140612679E-03
C	6.	9.6014125279E-05	-1.7673753000E-03	-9.0581230713E-04
H	1.	2.4969435846E-04	-6.4956326971E-04	-1.2277562388E-03
C	6.	-1.1058559763E-04	1.4458555474E-03	-2.2105915123E-04
H	1.	-9.0326566097E-04	-6.3346981015E-04	2.3470588533E-04
C	6.	-1.2352775931E-04	-1.7237080107E-03	1.4217507656E-03
H	1.	-1.4663255415E-04	1.7084880988E-04	-2.3317448394E-04
C	6.	6.5515224049E-04	8.5717682781E-04	3.9586737730E-05
H	1.	1.9488440758E-04	1.5438153127E-03	5.6508798556E-04
C	6.	-6.3461335813E-04	9.7344343976E-04	-5.5928271583E-04
C	6.	3.2255218693E-04	6.1468141625E-04	-1.0991200772E-03
C	6.	1.1028165932E-03	2.8534641681E-04	-7.1942624873E-04
C	6.	7.4088109320E-04	9.4020377962E-04	5.9094039190E-04
H	1.	-4.2936847657E-04	1.1197741261E-03	7.2362069406E-04
C	6.	-6.7788763463E-04	5.2441397813E-04	1.5377081834E-03
H	1.	4.8523977529E-04	-6.5847014650E-04	-4.0160717735E-04
C	6.	-1.1322840501E-03	7.4860077654E-04	1.3676435527E-03
H	1.	2.4638334335E-04	6.9892029587E-05	-1.3157152299E-03
C	6.	1.2178475045E-03	-2.1405357737E-03	3.6174350131E-04
H	1.	-2.5818162454E-04	2.5549705052E-05	9.9723875831E-05
C	6.	7.9078918670E-04	1.2315631711E-04	-9.0279855472E-04
C	6.	8.4596084356E-04	6.2408393270E-04	-1.7053447592E-03
C	6.	-4.0451871828E-04	-1.3861807290E-03	5.2373972441E-04
C	6.	5.9623386292E-04	1.5955501882E-03	-9.0070062324E-04
H	1.	-4.7373319945E-04	-1.1886277770E-03	1.2471120360E-03

C	6.	-4.7947631364E-04	-1.9239168108E-03	8.5552454231E-04
H	1.	-6.6663173097E-04	8.0175080344E-04	-8.1907875605E-04
C	6.	-1.7628030582E-04	2.0436189860E-03	-9.2881427868E-05
H	1.	-6.5773033464E-05	5.7441619893E-04	1.5800488663E-04
C	6.	5.9527642933E-04	-7.5297463054E-04	-2.1968971549E-04
H	1.	4.9179767679E-04	7.6544373036E-04	-2.2104207271E-04
C	6.	-9.0102852062E-05	2.8152114098E-04	-2.7531226402E-04
C	6.	8.7403106498E-04	-8.8310934656E-04	-7.8151702430E-04
H	1.	-4.2358808018E-04	-4.0282816589E-04	3.7947664647E-04
H	1.	-3.7546808240E-04	2.6171941126E-04	-6.6352726615E-04
C	6.	1.0719155204E-03	-8.0767404763E-04	-1.1029899730E-04
H	1.	-1.5496286624E-03	5.3862497318E-04	-1.5183632239E-03
H	1.	4.0059672610E-05	-5.9899015622E-04	-1.1343893214E-05
H	1.	-8.4727519133E-04	2.7273835103E-04	3.1454480879E-04

Table S7. DFT-optimized coordinates and gradient parameters for lowest excited triplet state of **3**.

COORDINATES OF SYMMETRY UNIQUE ATOMS (ANGS)

ATOM	CHARGE	X	Y	Z
RU	44.0	7.5334047283	3.2421528212	6.2702985219
O	8.0	5.8832557918	-0.2937356303	5.1629600235
N	7.0	9.0312771276	3.3276102940	5.0622503872
N	7.0	6.4962104742	1.9512106418	5.2224111940
O	8.0	9.2286689143	3.2449883369	3.9086572902
C	6.0	3.7491698258	2.5614428847	2.7824834341
H	1.0	3.0606317075	2.0200162827	2.1411062843
N	7.0	8.3090105521	1.4484572406	7.1109024599
C	6.0	7.6281289533	0.3883391925	6.6284034482
C	6.0	9.6117312592	-0.0036647948	8.4766100551
H	1.0	10.4163269195	-0.1126225073	9.1962731152
C	6.0	7.8834390692	-0.9036014421	7.0734955897
H	1.0	7.2855098716	-1.7130818866	6.6670699495
C	6.0	6.5677824461	0.6325415001	5.5767148692
C	6.0	9.2829816091	1.2597088750	8.0029497722
H	1.0	9.8104377486	2.1487101315	8.3342523762
C	6.0	8.8875840306	-1.0995608807	8.0136169493
H	1.0	9.1119160961	-2.0967687370	8.3778858019
O	8.0	6.2793215867	3.1359474604	7.7920269704
C	6.0	5.5456107531	2.5437565899	4.3848903955
C	6.0	4.6294710616	1.8472214787	3.5841249742
H	1.0	4.6191371038	0.7636232465	3.6117957841
C	6.0	4.9173411128	3.4726090069	7.7458517212
C	6.0	4.0432763879	2.2228635242	7.7248257073
O	8.0	5.8910285631	6.8201064641	5.1613696013
N	7.0	6.4549255245	4.5622424896	5.2657240219
C	6.0	3.7520653814	3.9605718307	2.7821580246
H	1.0	3.0684314982	4.5042850381	2.1375826879

N	7.0	8.3045103498	5.0594263829	7.1235017284
C	6.0	7.6194328087	6.1181985776	6.6397716069
C	6.0	9.6144294909	6.5225519416	8.4757698493
H	1.0	10.4189686886	6.6363307238	9.1949414525
C	6.0	7.8823797459	7.4128487557	7.0730506481
H	1.0	7.2836361557	8.2193827117	6.6598039258
C	6.0	6.5488507264	5.8784387400	5.5954290474
C	6.0	9.2864328711	5.2569799624	8.0080140385
H	1.0	9.8189472269	4.3721665895	8.3411321067
C	6.0	8.8879237761	7.6155908717	8.0088655608
H	1.0	9.1098995879	8.6148448130	8.3695700278
C	6.0	5.5369173024	3.9742025987	4.3968392717
C	6.0	4.6262157723	4.6735753739	3.5902603621
H	1.0	4.6213647081	5.7562824096	3.6200686838
H	1.0	4.6876794004	4.0817834902	8.6365815906
H	1.0	4.5084516933	1.4634042982	7.0918765535
H	1.0	3.0507512808	2.4406352127	7.3106217218
H	1.0	4.6738987609	4.0889184626	6.8688866725
H	1.0	3.9205365552	1.8038815327	8.7275523918

E= -1440.4140333416 GMAX= 0.0024107 GRMS= 0.0008711

RU	44.	6.1534477873E-04	3.9913936990E-05	1.9551262513E-04
O	8.	-1.7084835724E-04	1.7400680064E-03	7.4532755165E-04
N	7.	-5.0498062595E-04	3.5755599877E-04	1.2668277117E-03
N	7.	-2.7108933253E-04	-4.1060217489E-04	-8.5394208045E-04
O	8.	8.4977084982E-05	2.8141223354E-05	1.8131155851E-03
C	6.	-1.0587777002E-03	-8.3868217782E-04	2.7759698969E-04
H	1.	1.0644217873E-03	2.4430847499E-05	-1.7346533952E-04
N	7.	-8.7752177234E-04	1.8721416060E-05	1.3722197531E-04
C	6.	1.8593992506E-04	-1.0080012869E-03	-1.5904339094E-04
C	6.	3.9053213789E-04	-1.6128823692E-04	4.7638227211E-05
H	1.	3.5641131050E-04	7.9890106158E-04	-3.4700460809E-04
C	6.	7.9291474776E-05	-1.1579813823E-03	2.5899906718E-04
H	1.	-5.9643356804E-04	-2.8983578088E-04	1.3202239039E-04
C	6.	-6.8984386960E-04	-1.5201516493E-03	-5.9857353030E-04
C	6.	1.5528467759E-03	2.2907233513E-03	1.0261774919E-03
H	1.	7.9998220930E-04	5.9277732205E-04	-4.7460499885E-04
C	6.	-7.9490742066E-04	1.6196289224E-04	-2.5087203885E-04
H	1.	-7.8032338564E-05	7.9348162110E-04	-1.9840933729E-04
O	8.	-9.0505701701E-04	-1.7781566976E-03	-4.6950565854E-05
C	6.	-1.3248752956E-04	1.0069698338E-03	-9.6696843476E-04
C	6.	-2.2045913492E-04	-1.0444763657E-03	3.2430453892E-04
H	1.	-8.9815499972E-04	-1.3296837583E-03	5.5938103875E-04
C	6.	-1.6749103334E-03	-1.6431105475E-03	-1.4060211475E-04
C	6.	1.2770237682E-03	-4.5854900603E-04	-5.0394112592E-04
O	8.	-1.5639585122E-03	7.2490255331E-04	-3.5985538935E-04
N	7.	-9.8810545950E-05	-5.7827966978E-05	-1.0738725932E-03
C	6.	-6.2199016807E-04	1.0427174833E-03	6.0299826042E-04
H	1.	1.2109508412E-03	2.5422957370E-05	-4.1843938497E-06

N	7.	-1.1905690858E-03	-1.4751062863E-04	-4.8838862737E-04
C	6.	6.1179827363E-04	1.8974242651E-03	3.1664662829E-05
C	6.	2.4013071061E-04	6.5329008466E-04	-2.6021731756E-05
H	1.	2.9292271862E-04	-6.8014607746E-04	-1.8153827749E-04
C	6.	5.8560187274E-04	7.6917075998E-07	2.0675518583E-04
H	1.	-8.4203561120E-04	7.2397468109E-04	-1.0150969154E-04
C	6.	8.9093116770E-04	-9.5613519249E-04	-1.1586992160E-05
C	6.	2.3277800523E-03	-2.4106557042E-03	1.5793163019E-03
H	1.	6.8609431034E-04	-2.1598019318E-04	-4.7866208699E-04
C	6.	-6.3956319542E-04	-1.7916480269E-04	-2.9988050734E-04
H	1.	-2.4247903249E-04	-7.2023975476E-04	1.1206567846E-05
C	6.	8.8632128697E-04	-1.1397868509E-03	-3.5061633641E-04
C	6.	-1.0357257713E-03	2.2391810736E-03	-7.7278061194E-04
H	1.	-4.2571090298E-04	6.4306448244E-04	1.9169516048E-04
H	1.	9.3714507114E-04	3.5010893039E-04	1.2524277398E-03
H	1.	1.4873536137E-03	7.9120754440E-04	1.0238377486E-03
H	1.	2.4190408064E-04	-2.4007914282E-04	-1.7916995357E-03
H	1.	-7.1518650718E-04	-2.0997949011E-04	-4.1591196210E-04
H	1.	-5.5617191984E-04	1.6523141307E-03	-6.1314051779E-04