Electronic Supplementary Information (ESI)

Ru^{III}(edta)-Mediated Interaction of Nitrite and Sulphide: Formation of N-bonded Thionitrous acid (HSNO) Complex of Ru^{III}(edta) in Aqueous Solution

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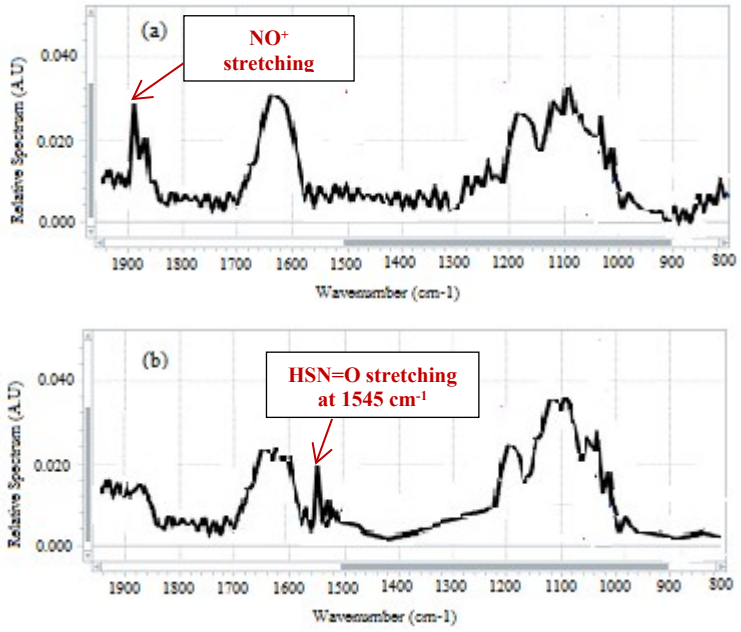

Figure S1. IR spectra of (a) [Ru^{III}(edta)(NO^+)] in solution and (b) the resultant soution that was obtained by reacting [Ru^{III}(edta)(NO^+)] with NaHS leading to the formation of N-bonded [Ru^{III}(edta)(N(O)SH]$^-$.

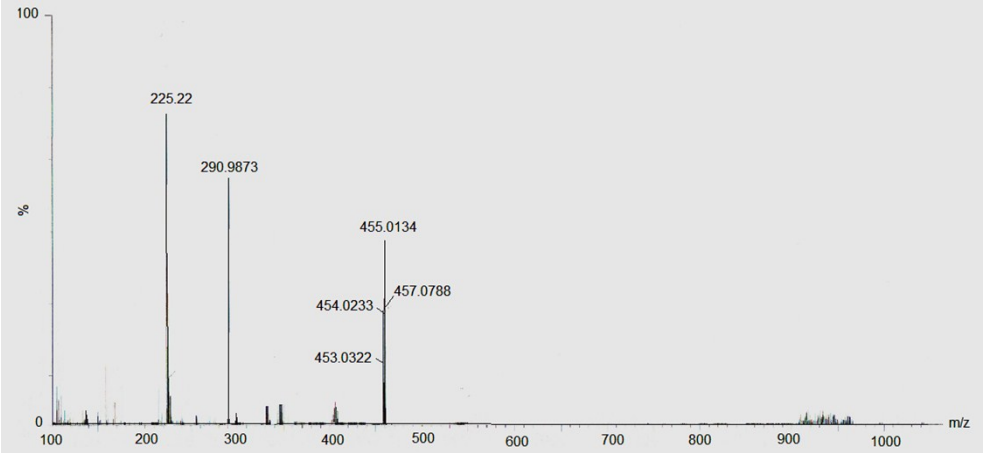

Figure S2. ESI-MS spectrum recorded for the resultant solution that was obtained after addition of NaHS to the solution of [Ru^{III}(edta)(NO^{+})]. [Ru^{III}] = 0.2 mM, [NaHS] = 0.5 mM, pH 3.5 (acetate buffer) under Ar atmosphere.

Table S1. The corresponding important Ru-N and Ru-O bond-lengths for all the N- and S-bonded structures.

System	Bonds	Bond-length (Å)
I	Ru-N_1	2.11
	Ru-N_2	2.24
	Ru-O_a	2.00
	Ru-O_b	2.00
	Ru-O_c	2.01
II	Ru-N_1	2.09
	Ru-N_2	2.24
	Ru-O_a	1.99
	Ru-O_b	2.01
	Ru-O_c	2.07
III	Ru-N_1	2.13
	Ru-N_2	2.27
	Ru-O_a	2.03
	Ru-O_b	2.02
	Ru-O_c	2.07
IV	Ru-N_1	2.10
	Ru-N_2	2.17
	Ru-O_a	2.04
	Ru-O_b	2.02
	Ru-O_c	2.08
V	Ru-N_1	2.17
	Ru-N_2	2.20
	Ru-O_a	2.08
	Ru-O_b	2.05
	Ru-O_c	2.06
VI	Ru-N_1	2.16
	Ru-N_2	2.19
	Ru-O_a	2.06
	Ru-O_b	2.07
	Ru-O_c	2.09

Table S2. Cartesian coordinates, low vibrational frequencies and energies in atomic unit (a.u.) for the optimized structures **I-VI**.

Structure I

Low frequencies (cm^{-1}): 26.48 30.55 44.90

Ru	0.59521000	-0.23304100	-0.13257900
O	4.37244000	0.87414200	0.65632500
O	2.59783400	-0.23851000	-0.16135000
O	-0.03692600	2.74342600	-2.76348800
O	0.26738600	0.69903600	-1.88017200
O	-0.72565000	-1.36405800	3.58754100
O	0.55061500	-0.92258300	1.79001500
O	-4.35113400	0.57378800	0.56392400
O	-4.75045000	-0.33794600	-1.45774400
N	0.88698000	1.72935300	0.59940400
N	-1.55951900	0.09397600	0.38208100
C	-0.29735500	2.02253600	1.45384300
C	-1.58619100	1.55225100	0.77120200
C	2.18855500	1.63826800	1.32526000
C	3.17608200	0.72852700	0.55883200
C	0.98336700	2.62297000	-0.59780900
C	0.33714300	2.02466500	-1.86125300
C	-1.83572000	-0.81508200	1.53811600
C	-0.59717800	-1.05442900	2.41960100
C	-2.46281000	-0.18243900	-0.76814800
C	-3.96861600	-0.00152100	-0.60293100
H	-0.37287900	3.09994200	1.65611500
H	-0.15276300	1.51339100	2.40787600
H	-1.74923100	2.12489600	-0.14635900
H	-2.43864200	1.74499600	1.42844600
H	2.00435600	1.16574100	2.29397000

H	2.63577500	2.62478400	1.48281400
H	2.04242200	2.77696000	-0.82693800
H	0.54663600	3.60406200	-0.38757200
H	-2.12552900	-1.78672000	1.12590900
H	-2.66239900	-0.44126800	2.14620300
H	-2.30037000	-1.21804500	-1.07340600
H	-2.14544500	0.43543700	-1.61336400
N	0.44361200	-2.10944300	-0.89671600
O	-0.59115700	-2.72556500	-1.03696100
S	1.90263300	-2.97913700	-1.41148500
H	2.72869100	-1.97720800	-1.00862400
H	-5.32682600	0.62749800	0.53379200

Energy = -1722.8368147

Structure II

Low frequencies (cm^{-1}): 8.22 24.30 38.49

Ru	0.54038800	-0.01760200	0.35317700
O	4.25458300	-1.16987600	-0.57903100
O	2.51980200	-0.23312700	0.50264400
O	-0.66343400	-3.65999200	1.56292000
O	-0.07308800	-1.48971000	1.58169700
O	-0.26500700	2.71712500	-2.63798800
O	0.77649400	1.42463500	-1.11955300
O	-4.36850700	0.08495300	-0.84845100
O	-4.83616100	0.51397100	1.31404000
N	0.71852000	-1.55744400	-1.05414100
N	-1.56600400	0.17528400	-0.38169100
C	-0.39380500	-1.35152500	-2.02326900
C	-1.69777400	-1.02124400	-1.29013800

C	2.09045900	-1.36175900	-1.60926200
C	3.07118400	-0.92562500	-0.49220000
C	0.60807400	-2.84629900	-0.29867400
C	-0.12264500	-2.70135600	1.05007000
C	-1.63208700	1.46866700	-1.12934600
C	-0.28021200	1.92183600	-1.71662700
C	-2.53686600	0.13662400	0.74326400
C	-4.02864700	0.27547700	0.44979700
H	-0.54339300	-2.24920200	-2.63926900
H	-0.10571100	-0.53486100	-2.68768600
H	-2.00163200	-1.86800200	-0.66823000
H	-2.49489100	-0.85308200	-2.01985000
H	2.04854500	-0.54662700	-2.33688200
H	2.46057500	-2.26690300	-2.10091200
H	1.62014000	-3.19756700	-0.07529800
H	0.11864900	-3.61270600	-0.90744000
H	-1.93946000	2.24513800	-0.42026400
H	-2.38591100	1.42906900	-1.92001100
H	-2.28459200	0.94084700	1.43805200
H	-2.38555600	-0.79445500	1.29847500
H	-5.33969000	0.18682900	-0.89397300
S	0.61152700	1.73715600	2.06586300
H	1.73698500	1.29865800	2.67866000
N	1.70536900	3.08930100	0.78879800
O	2.83821300	2.97253200	0.85979400

Energy = -1722.8182998

Structure III

Low frequencies (cm^{-1}): 39.79 44.43 46.50

Ru	0.52136500	-0.15076500	-0.31862000
O	4.41260000	0.29223100	0.72638700
O	2.54934200	-0.33878300	-0.36516700
O	0.62708200	3.55568800	-1.94507200
O	0.43825000	1.32756900	-1.69614100
O	-0.66761400	-2.43019800	2.90342000
O	0.53369000	-1.54627800	1.22229000
O	-4.20825000	0.64287900	1.05769100
O	-4.79691100	0.55821000	-1.14607400
N	1.02655600	1.42881600	1.01636000
N	-1.50275500	0.11042000	0.42608500
C	-0.12475100	1.53681600	1.95929000
C	-1.43474400	1.40399300	1.19485000
C	2.30261000	0.98493700	1.64024400
C	3.20112300	0.28182800	0.59548200
C	1.21610300	2.65676800	0.18025300
C	0.70724500	2.54094900	-1.27486000
C	-1.81765200	-1.05045100	1.31664300
C	-0.57778600	-1.73138400	1.90769500
C	-2.52566700	0.23316700	-0.66372400
C	-4.02475100	0.51380100	-0.17455600
H	-0.09590900	2.49773100	2.49292600
H	-0.02113900	0.74111800	2.70080800
H	-1.52100200	2.20978900	0.45994400
H	-2.31435000	1.46355900	1.84034700
H	2.06383900	0.24224700	2.40638200
H	2.84111600	1.81983400	2.10217500
H	2.28732800	2.87121800	0.11965700

H	0.73950700	3.51976100	0.65590800
H	-2.32210300	-1.80257400	0.70114900
H	-2.52836700	-0.75292700	2.08762300
H	-2.52049700	-0.69777400	-1.23422300
H	-2.20852600	1.03337900	-1.33562900
N	0.19425100	-1.59298700	-1.67349100
O	-0.32864000	-1.45825100	-2.74842600
S	0.84448200	-3.26457400	-1.34194700
H	1.11521300	-2.94935900	-0.04845700

Energy = -1722.3180916

Structure IV

Low frequencies (cm^{-1}): 24.30 42.99 44.85

Ru	0.52106500	0.04064300	0.38238500
O	4.39342700	-0.39378100	-0.70204900
O	2.55795300	0.20045800	0.45961000
O	0.57034300	-3.79156300	1.68807300
O	0.39238000	-1.54828100	1.63501300
O	-0.62814000	2.50145100	-2.71068100
O	0.53470300	1.57546300	-1.02563200
O	-4.24747500	-0.54339800	-0.99621000
O	-4.82950000	-0.56168600	1.20946200
N	0.97090400	-1.40564500	-1.07239800
N	-1.52018400	-0.10498800	-0.34789300
C	-0.18847600	-1.41695300	-2.01455300
C	-1.48980700	-1.32811000	-1.22681100
C	2.25504400	-0.92566500	-1.65887100
C	3.18336600	-0.35248200	-0.55731000
C	1.14922200	-2.70955500	-0.35362600
C	0.65126900	-2.72182500	1.10914500
C	-1.81698200	1.12859200	-1.14007600

C	-0.56254700	1.78975600	-1.71951900
C	-2.54789600	-0.29130400	0.73241300
C	-4.05250000	-0.48891600	0.24246600
H	-0.17570800	-2.33061600	-2.62577300
H	-0.07720400	-0.56449900	-2.68865700
H	-1.58412300	-2.19369700	-0.56410400
H	-2.37759000	-1.31606600	-1.86399300
H	2.02455900	-0.10238500	-2.34050000
H	2.76828200	-1.72136900	-2.20993300
H	2.21773500	-2.94246600	-0.32248500
H	0.65682400	-3.51692500	-0.90431200
H	-2.26227400	1.85514900	-0.45149400
H	-2.56779500	0.91630900	-1.90124200
H	-2.50997500	0.59255300	1.37513000
H	-2.24424100	-1.14972700	1.33636900
S	0.33442000	1.72684700	2.10909500
H	1.66561100	1.90736500	2.29643400
N	0.19557700	3.39607800	0.89833400
O	1.15382200	4.04248800	0.87594100

Energy = -1722.2974927

Structure V

Low frequencies (cm^{-1}): 46.26 49.08 52.64

Ru	0.56744600	-0.35187500	-0.31033500
O	4.53558600	-0.30491100	0.69926400
O	2.59740900	-0.80735800	-0.33559800
O	1.14521800	3.22490800	-2.20375600
O	0.53847000	1.09911200	-1.77068100
O	-0.86320700	-1.93019700	3.21623000
O	0.41101900	-1.46021000	1.42821300
O	-3.98342400	1.39367700	1.08576500

O	-4.66592400	1.25576200	-1.07785300
N	1.33550700	1.27932100	0.89499600
N	-1.40750700	0.31113600	0.41160100
C	0.22216400	1.64367500	1.80821300
C	-1.10926600	1.63355500	1.06245200
C	2.52915400	0.69621600	1.55146800
C	3.31946400	-0.19762600	0.55903000
C	1.69910800	2.36313600	-0.05601600
C	1.06834200	2.24770000	-1.46574600
C	-1.86121000	-0.71091600	1.40457900
C	-0.70417900	-1.42380400	2.10730400
C	-2.47403200	0.52234100	-0.63204500
C	-3.85391500	1.12208800	-0.13924400
H	0.38916000	2.64271400	2.24486800
H	0.21469700	0.92110800	2.62702700
H	-1.08218000	2.37568500	0.25843100
H	-1.95455900	1.89282200	1.70618400
H	2.18037900	0.04341900	2.35604300
H	3.19046100	1.46910700	1.96620000
H	2.78362500	2.33904800	-0.20384400
H	1.45149300	3.34681600	0.36220500
H	-2.38401600	-1.48470800	0.83496200
H	-2.56674200	-0.26299400	2.10589100
H	-2.65221800	-0.44836900	-1.10055300
H	-2.04866300	1.17723000	-1.39728600
N	0.03766300	-1.86996300	-1.57844800
O	0.72931800	-1.90486000	-2.59608900
S	-1.17613800	-3.02990000	-1.31039900

Energy = -1721.7241039

Structure VI

Low frequencies (cm^{-1}): 16.62 39.79 48.09

Ru	0.54036600	0.34843000	-0.18741800
O	4.53357800	-0.53349600	-0.46817300
O	2.58023100	0.59427500	-0.48178000
O	1.00894800	0.04688800	3.86618900
O	0.54255900	0.85577000	1.81447400
O	-0.76107600	-1.74006100	-3.50741000
O	0.46417500	-0.46609000	-2.11733600
O	-4.03539700	-1.71768800	0.29558000
O	-4.74374300	0.19390500	1.30165300
N	1.26649900	-1.54389500	0.56905900
N	-1.42026100	-0.61463200	-0.11933700
C	0.17038500	-2.51289600	0.30937200
C	-1.17895400	-1.88864500	0.64069900
C	2.50492000	-1.79143600	-0.20839300
C	3.30893200	-0.47814300	-0.38381400
C	1.55035600	-1.34360900	2.01780700
C	0.97430200	-0.04544600	2.64182600
C	-1.82103400	-0.87269600	-1.53691000
C	-0.62719900	-1.07476000	-2.48009300
C	-2.50184100	0.16575500	0.58600200
C	-3.91062400	-0.54302100	0.73636100
H	0.31184100	-3.42862800	0.90705600
H	0.21893900	-2.79442700	-0.74503900
H	-1.20879000	-1.62641500	1.70299400
H	-2.01800800	-2.56475500	0.45548500
H	2.20966800	-2.11594200	-1.21021700
H	3.13390700	-2.56240600	0.25602400

H	2.63573900	-1.29272400	2.15139400
H	1.19381600	-2.20041900	2.60172000
H	-2.34016100	0.02778200	-1.88141600
H	-2.53191500	-1.69885700	-1.58052300
H	-2.62612100	1.10219100	0.03826300
H	-2.11776300	0.42810500	1.57555900
S	-0.14440600	2.44285200	-1.13998500
N	-0.15591800	3.65868500	0.15967600
O	-0.46108200	4.78127500	-0.20170600

Energy = -1721.7194183

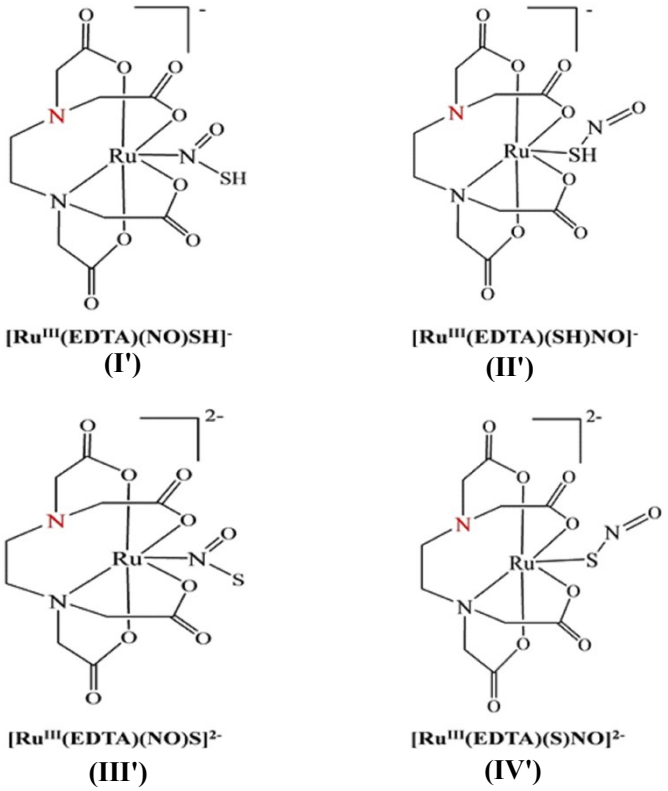

Figure S3. Pictorial representations of different HSNO/SNO^{-} complexes of Ru^{III}(edta) wherein all four carboxylate groups and one N-atom of the ethylenediamine collar are coordinated.

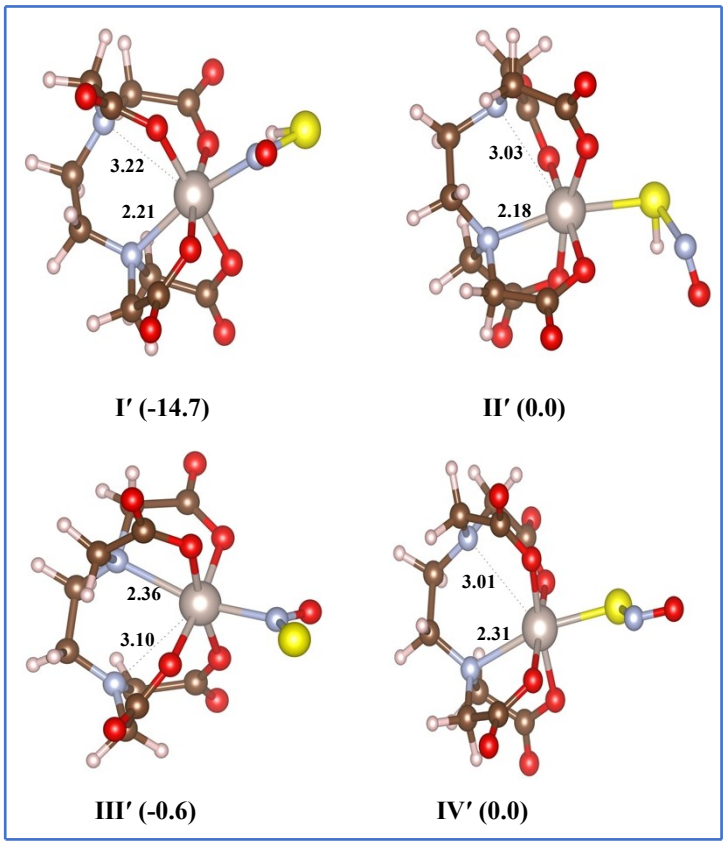

Figure S4 Optimized structures of I'-IV' which correspond to four -COO bonded and one –NH2 bonded Ru configurations. The numbers correspond to the important bond-lengths in the molecules.

Table S3. Cartesian coordinates, low vibrational frequencies and energies in atomic unit (a.u.) for the optimized structures **I'-IV'**.

Structure I'

Low frequencies (cm^{-1}): 19.90 36.45 36.63

Ru	-0.23399000	-0.45402200	0.29961500
N	1.57161600	2.12234100	-0.40056300
N	-1.23233100	1.01355100	-1.02627200
O	-4.12370400	0.32170600	1.11635700
O	3.74366100	-0.62783800	-1.38682600
O	1.61453100	-0.69695100	-0.71606300
O	-2.03975500	-0.51108100	1.17037900
O	-0.91965100	-1.65324000	-1.20522800

O	0.41513100	0.71515700	1.83722400
N	0.33121200	-2.01401100	1.44721400
H	0.66096800	3.90538800	-1.08444500
H	-1.50824700	3.04213500	-1.56678300
H	0.80515100	2.60487500	-2.26443300
H	-1.10793400	2.74299900	0.12987700
C	0.59401200	2.80528300	-1.20934500
C	-0.86468700	2.44856500	-0.89611400
H	2.76978200	1.77858200	-2.08392900
H	-3.19421900	1.83579900	-0.74519500
H	2.69914300	2.32044900	1.32998300
H	-1.59925800	0.89950900	-3.13960200
H	0.08845800	0.64166200	-2.62972000
H	1.60192300	3.67661300	1.03177100
C	1.69877600	2.58080700	0.96253500
C	-0.95518200	0.44940400	-2.37258200
C	2.69932100	1.47707000	-1.02939000
C	-2.69407000	0.86397100	-0.70541900
H	3.64510200	1.79160200	-0.56824700
H	-3.15823700	0.23285900	-1.46959500
O	-1.45238400	-1.66273100	-3.39135300
O	0.32006700	2.68347800	2.90985600
C	2.71134200	-0.06768900	-1.03304200
C	-3.00293300	0.20292300	0.64797400
C	-1.14216800	-1.08263200	-2.36242400
C	0.70079800	1.98032100	1.98189200
O	-0.13407900	-2.24089600	2.52909600

H	1.84286000	-2.36314300	-0.20705600
S	1.51217600	-3.22215700	0.82060300

Energy = -1722.3224248

Structure II'

Low frequencies (cm^{-1}): 21.24 30.99 37.72

Ru	-0.31195800	-0.08389800	-0.28873800
N	2.58212100	-0.37249600	0.56536500
N	0.23205100	1.47472100	1.14639300
O	-2.85602100	0.39801800	2.84573700
O	3.05818900	0.62092600	-2.83155500
O	1.12771700	0.37828200	-1.72471200
O	-1.89585300	-0.35728000	0.95886700
O	-1.29742400	1.53439000	-1.06472000
O	0.32889600	-1.94269500	0.41595500
H	3.56480100	0.96216300	1.91297600
H	1.64507000	2.25155500	2.51797600
H	2.94155200	1.65847000	0.42226000
H	1.23939300	0.54073800	2.71322700
C	2.71966200	0.91574900	1.19509400
C	1.45982500	1.31287900	1.97041300
H	4.21759200	-0.25630400	-0.80795100
H	-0.63633700	1.69033900	3.09354400
H	3.38958800	-2.19458800	1.29703200
H	0.33568000	3.59876700	0.87391600
H	1.23076000	2.62103900	-0.32191900
H	2.50643500	-1.23864500	2.46740300
C	2.51255100	-1.53903400	1.41231600
C	0.31639400	2.68110100	0.27196700

C	3.15389300	-0.54208600	-0.74919500
C	-0.96387700	1.59482000	2.05480500
H	3.09167800	-1.60565700	-1.00765500
H	-1.50555600	2.51294400	1.80751000
O	-1.29509100	3.78549200	-1.12173300
O	1.23243100	-3.51846400	1.72932100
C	2.40987500	0.22755600	-1.86491000
C	-1.99497300	0.44763400	1.98001200
C	-0.86278600	2.71662300	-0.71634900
C	1.25859700	-2.41811900	1.18481400
N	-2.89083800	-2.21724900	-0.83132100
H	-2.10772900	-0.56472900	-2.56798100
O	-3.91666700	-1.73662800	-1.07390800
S	-1.34965400	-1.50990500	-1.95992100

Energy = -1722.299023

Structure III'

Low frequencies (cm^{-1}): 34.84 38.35 42.99

Ru	-0.39968700	-0.35990400	0.25018700
N	2.43918200	0.60245900	-0.54675500
N	-0.27012300	1.89809600	-0.43675100
O	-1.77546800	2.52781100	2.83412200
O	1.65477000	-1.28383500	-3.37725700
O	0.37610500	-1.11812400	-1.53964300
O	-1.22639600	0.56098200	1.89277000
O	-2.15141800	-0.02328800	-0.78795600
O	1.24860700	-0.82946500	1.48552300
N	-1.03359700	-2.19093300	0.88078100
H	3.01426500	2.52676900	-1.28811800
H	0.87677800	3.58645500	-1.02473700
H	1.85658500	1.60923400	-2.24787200
H	1.32344900	2.83246100	0.51101900
C	2.14199200	1.83805700	-1.21548100
C	1.01624200	2.61251000	-0.51646300
H	3.56210100	-0.41446000	-2.05916000
H	-0.80891400	3.59259600	0.75833500
H	4.12960200	0.43285600	0.74300100
H	-1.19256500	2.78875300	-2.15449000
H	-0.24799600	1.30364600	-2.45865700
H	2.94394000	1.65438600	1.17782900
C	3.04459100	0.64582700	0.75796800
C	-0.92786500	1.79528700	-1.75797000
C	2.71923600	-0.55922000	-1.35823400

C	-1.16828700	2.57979800	0.54098700
H	2.98277100	-1.37942200	-0.68111300
H	-2.16115900	2.68991900	0.09209200
O	-3.14779300	1.17981300	-2.40939000
O	3.05244100	-0.56780800	2.79718900
C	1.49142400	-1.01987100	-2.18016500
C	-1.38919100	1.84514200	1.88424700
C	-2.19892800	0.92782800	-1.66759700
C	2.39936800	-0.33014900	1.77588900
O	-1.04032900	-2.37119500	2.09048900
S	-1.58353200	-3.38532200	-0.19519600

Energy = -1721.6998154

Structure IV'

Low frequencies (cm^{-1}): 23.62 28.99 40.42

Ru	0.42631100	-0.16144800	-0.21114600
N	-1.86247800	1.68505200	0.46542800
N	-1.39582800	-1.27355600	0.68943200
O	1.08889200	-2.56828900	3.05124400
O	-2.11203000	1.82890600	-3.06641700
O	-0.63248900	0.64233300	-1.86480100
O	1.36659600	-1.14244900	1.33278500
O	0.32350600	-1.92243800	-1.30173300
O	0.83039100	1.57730300	0.93548100
H	-3.78952200	1.15116200	1.22825700
H	-3.31455900	-1.17458600	1.59579700
H	-3.32963100	0.46855400	-0.32969000

H	-2.03718000	-0.22085700	2.36296500
C	-2.93022400	0.73919800	0.65325300
C	-2.44872500	-0.51595200	1.39263800
H	-2.77166200	2.98415500	-0.97291600
H	-1.38541200	-2.39956600	2.51056300
H	-1.69144200	3.41494500	1.69519600
H	-2.65786200	-2.73630700	-0.23673500
H	-2.42190900	-1.21984200	-1.15002300
H	-1.72658900	1.87594800	2.53995900
C	-1.35390200	2.36554000	1.63168500
C	-1.92955900	-1.95735200	-0.51124000
C	-1.83493100	2.43294300	-0.77104400
C	-0.76985200	-2.26578100	1.61358500
H	-1.02819000	3.17059000	-0.68921800
H	-0.73096500	-3.23881100	1.11250700
O	-1.00723200	-3.61120300	-1.97712000
O	0.69284400	3.13924400	2.54971900
C	-1.51881500	1.56540100	-2.01365900
C	0.67994500	-1.95875300	2.06182400
C	-0.79009700	-2.57980000	-1.34020800
C	0.19534500	2.36555000	1.72371200
N	3.75030100	0.47808300	-0.34228100
O	4.81435300	0.78276300	-0.86602100
S	2.37309600	0.49037000	-1.44079100

Energy = -1721.6980112

Table S4. Cartesian coordinates, low vibrational frequencies and energies in atomic unit (a.u.) for the optimized transition state (TS) structures.

Structure transition state (TS)

Imaginary frequency (cm^{-1}): -248.7474

Ru	0.53611400	0.03284000	0.30254200
O	4.41170000	-0.46978300	-0.74530700
O	2.58148100	0.17562600	0.40170700
O	0.47182400	-3.75676400	1.71009500
O	0.32664600	-1.51025000	1.60808300
O	-0.59774900	2.50967200	-2.77592600
O	0.58455300	1.47189900	-1.17117700
O	-4.23644100	-0.51600100	-1.00701800
O	-4.79844800	-0.46071700	1.20371500
N	0.97090800	-1.41702000	-1.07496200
N	-1.50551500	-0.09374000	-0.40363100
C	-0.18892600	-1.45825000	-2.02699600
C	-1.49527000	-1.33539000	-1.25268000
C	2.26278800	-0.97616000	-1.68972800
C	3.20248700	-0.39999200	-0.60000000
C	1.14745700	-2.70962400	-0.32016300
C	0.58849600	-2.69725400	1.11940300
C	-1.78772800	1.13237800	-1.21438200
C	-0.52407800	1.76559500	-1.80968400
C	-2.51656800	-0.23690500	0.69585600
C	-4.03114600	-0.42600000	0.22726800
H	-0.16504900	-2.39486700	-2.59991200
H	-0.06492000	-0.62996400	-2.72701000
H	-1.61042500	-2.18520800	-0.57324900

H	-2.37566600	-1.32343400	-1.89976000
H	2.03899900	-0.16578900	-2.38728100
H	2.74458100	-1.80356600	-2.22086000
H	2.21974500	-2.90879000	-0.24007200
H	0.69811200	-3.53388800	-0.88141100
H	-2.22508300	1.87324900	-0.53793900
H	-2.54065200	0.91646300	-1.97267600
H	-2.45337500	0.66348700	1.31259400
H	-2.22014400	-1.08674200	1.31500000
S	0.94295600	1.65458100	3.03247700
H	1.94677400	2.56050500	2.95099300
N	-0.03399100	2.34811800	1.56917900
O	0.30316600	3.40117000	1.15627000

Energy: -1722.2709623