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Supporting Information: The Bonding Situations in Ruthenium Chalcogenonitrosyl Compounds: A Physical Reasoning

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Frontier Molecular Population Analysis

In the frontier molecular orbitals for oxidized species, the contribution from the cobalt center in **1a** was observed to persist following the replacement of oxygen by other chalcogen atoms (**2a**-**4a**). The analysis of the adjacent orbitals indicates that the HOMO-1 behaves similarly for all oxidized compounds, whereas the HOMO-2 for **1a** exhibits a distinct pattern compared to **2a**, **3a**, and **4a**. The HOMO-1 orbitals are constituted by the combination of the p(Cl)/d(Ru)/π(NE), while for the HOMO-2, **1a** has a contribution solely from p(Cl), whereas **2a**-**4a** have the same contributions as HOMO-1.

The lowest unoccupied molecular orbital (LUMO) and LUMO+1 orbitals are composed of d(Ru)/π^*(NE) and **1a** has a small contribution from d(Co). The LUMO+2 has a major contribution from the d(Co) and p(PO) groups *trans* to chloride's, as well as the π orbitals of cyclopentadienyl. Again, **1a** shows different behavior compared to **2a**-**4a**, which have contributions from d(Ru)/π^*(NO).

The Frontier Molecular Orbital Population analysis (FMOP) by Löwdin charges (Table S3) show that in the HOMO orbital, ruthenium exhibits approximately 0.56, while Cl_1 0.17, Cl_2 ca. 0.18 and the L_{OEt}^- ca. 0.09 contribution, with energies of -4.64, -4.60, -4.63 and -4.65 eV for **1a**-**4a**, respectively. In the LUMO orbital, **1a** exhibits different behavior compared to **2a**-**4a**. The ruthenium contribution is 0.25, 0.32, 0.34 and 0.35 for **1a**-**4a**, and the chalcogenonitrosyl contributes 0.47, 0.60, 0.58 and 0.57 for **1a**-**4a**, respectively. The main difference is the contribution of L_{OEt}^-, which is 0.27 for **1a**, while in **2a**-**4a** the contribution is approximately 0.05. The energy of the LUMO orbital is -2.91, -3.39, -3.40 and -3.48 eV for **1a**-**4a**, respectively.

Differently, the HOMO-1 have the main contribution from d(Ru)/π(NE) and for **1b**-**2b** have the contribution from two chlorides. For **3b**-**4b** have the contribution of just one chloride. It is also possible to observe that as the size of the chalcogen increases, its contribution from the atomic orbital to the formation of the molecular orbital also increases.

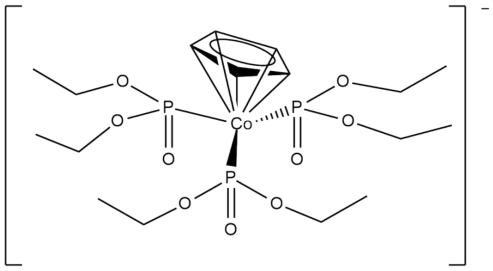
The analysis of lowest unoccupied molecular orbital for reduced complex show the same

contribution for LUMO, LUMO+1 and LUMO+2, with exception of NO in LUMO+2 which have the contribution from p(Cl). The LUMO and LUMO+1 orbitals is located mainly in L_{OEt}^{-} portion and the LUMO+2 have the contribution from d(Co)/π^*(NE).

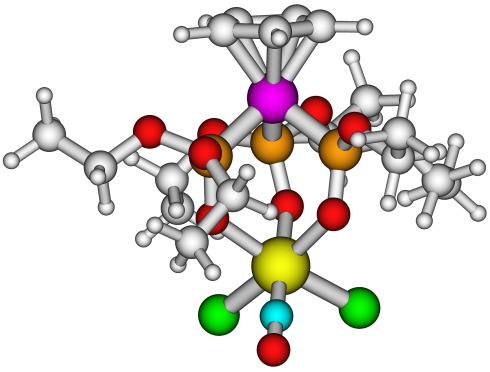
The Löwdin charge (Table S3) for the frontier molecular orbital, show the principal contribution from Ru and NE in the SOMO orbital. For the **1b** ruthenium is 0.48 and NO 0.39. Interestingly, going from S to Te the contribution of ruthenium down to ca. 0.40 and the NE increase to ca. 0.49. The chlorides ligand contribute only with 0.02 and the L_{OEt}^{-} ca. 0.07. For the LUMO, the Löwdin charge show the mainly contribution is from L_{OEt}^{-}, with value of 0.99. The SOMO energies is -0.16, -0.14, -0.43, and -0.61 eV for **1b-4b**, respectively, and the LUMO energies is 0.12, 0.10, 0.02, and -0.04 for **1b-4b**, respectively. So, conform the chalcogen increase, the SOMO and LUMO is stabilized, mainly in the energy of SOMO orbitals.

The difference between the energy of frontier molecular orbitals in oxidized species have a different behavior from reduced species. For **1a-4a** the difference is 1.73, 1.21, 1.23, and 1.17 eV, respectively and for **1b-4b** the difference is 0.28, 0.24, 0.45, and 0.57 eV, respectively.

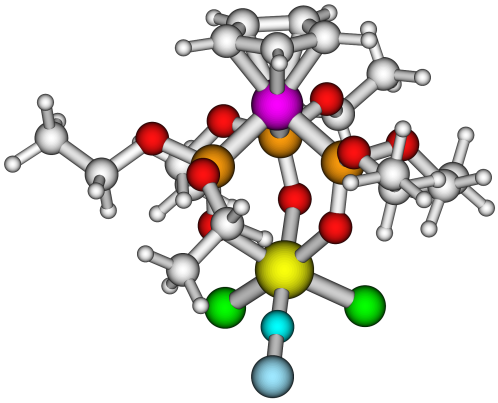
Figures and Tables



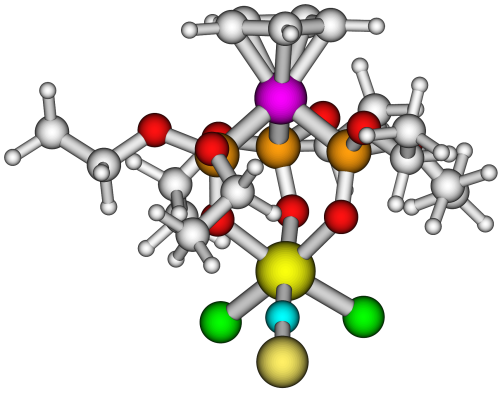
L_{OEt}^-



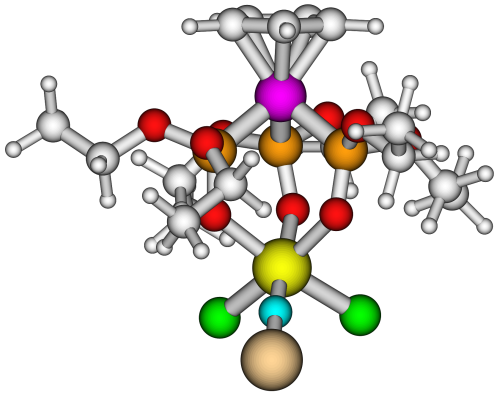
(**1a**)



(**2a**)

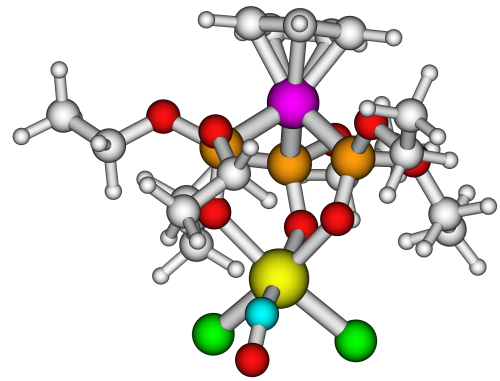


(**3a**)

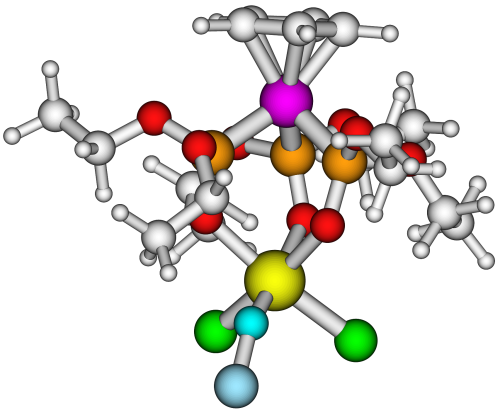


(**4a**)

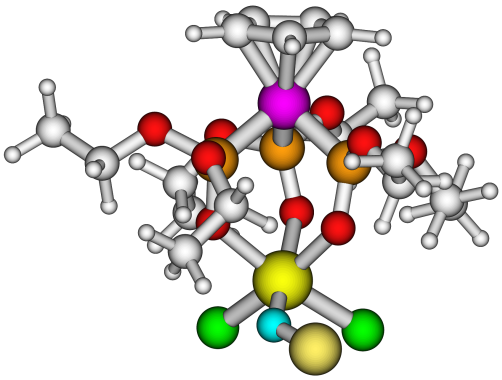
Figure S1: 2D chemical structure of the ligand L_{OEt}^-. Optimized geometries of ruthenium chalcogenonitrosyl complexes in the oxidized form ($\{N{-}E\}^+$)(**1a**-**4a**) (E= O, S, Se, Te), color code: C = gray, H = white, Cl = green, P = orange, O = red, N = cyan, S = blue-green, Se = pale yellow, Te = beige, Co = purple, Ru = yellow.



(**1b**)



(**2b**)



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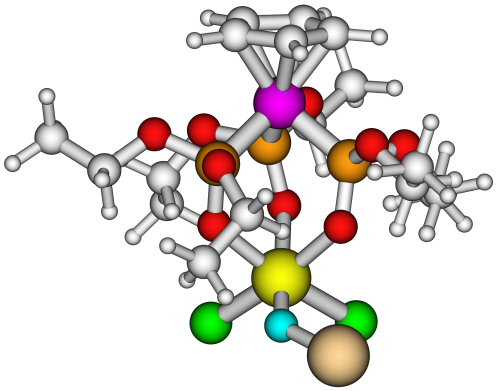


(**4b**)

Figure S2: Optimized geometries of ruthenium chalcogenonitrosyl complexes in the reduced form ($\{N{-}E\}^0$) (**1b-4b**) (E= O, S, Se, Te), color code: C = gray, H = white, Cl = green, P = orange, O = red, N = cyan, S = blue-green, Se = pale yellow, Te = beige, Co = purple, Ru = yellow.

Table S1: Löwdin Atomic Charges ($q^{Löwdin}$) and Bond Orders ($b_{AB}^{Löwdin}$) for componds **1a-4b**.

Atom/Bond	$q^{Löwdin}$		Bond	$b_{AB}^{Löwdin}$	
	1a	**1b**		**1a**	**1b**
Ru	-0.381	-0.536	Ru−N	2.177	1.921
N	-0.061	-0.129	N−O	2.648	2.495
O	0.151	0.005	Ru−Cl_1	1.323	1.286
Cl_1	-0.019	-0.097	Ru−Cl_2	1.316	1.287
Cl_2	-0.017	-0.092	Ru−O_1	0.643	0.432
O_1	-0.132	-0.151	Ru−O_2	0.633	0.556
O_2	-0.146	-0.137	Ru−O_3	0.692	0.553
O_3	-0.130	-0.129	P_1−O_1	1.906	1.997
N−O	0.090	-0.280	P_2−O_2	1.896	1.988
P_1−O_1	0.191	0.166	P_3−O_3	1.868	2.068
P_2−O_2	0.171	0.188	—	—	—
P_3−O_3	0.194	0.197	—	—	—
	2a	**2b**		**2a**	**2b**
Ru	-0.384	-0.532	Ru−N	2.102	1.874
N	-0.270	-0.324	N−S	2.458	2.281
S	0.360	0.119	Ru−Cl_1	1.333	1.302
Cl_1	-0.002	-0.074	Ru−Cl_2	1.329	1.301
Cl_2	-0.003	-0.074	Ru−O_1	0.643	0.563
O_1	-0.130	-0.128	Ru−O_2	0.632	0.558
O_2	-0.142	-0.137	Ru−O_3	0.651	0.486
O_3	-0.135	-0.146	P_1−O_1	1.904	1.983
N−S	0.090	-0.205	P_2−O_2	1.897	1.977
P_1−O_1	0.193	0.198	P_3−O_3	1.890	2.034
P_2−O_2	0.179	0.185	—	—	—
P_3−O_3	0.184	0.180	—	—	—

Atom/Bond	$q^{Löwdin}$		Bond	$b_{AB}^{Löwdin}$	
	3a	**3b**		**3a**	**3b**
Ru	-0.371	-0.497	Ru−N	2.158	1.998
N	-0.237	-0.267	N−Se	2.303	2.025
Se	0.306	-0.002	Ru−Cl_1	1.330	1.307
Cl_1	0.000	-0.057	Ru−Cl_2	1.329	1.284
Cl_2	0.001	-0.088	Ru−O_1	0.644	0.553
O_1	-0.129	-0.125	Ru−O_2	0.632	0.601
O_2	-0.140	-0.118	Ru−O_3	0.641	0.461
O_3	-0.137	-0.148	P_1−O_1	1.903	1.992
N−Se	0.069	-0.269	P_2−O_2	1.897	1.958
P_1−O_1	0.194	0.195	P_3−O_3	1.894	2.047
P_2−O_2	0.179	0.206	—	—	—
P_3−O_3	0.182	0.167	—	—	—
	4a	**4b**		**4a**	**4b**
Ru	-0.346	-0.461	Ru−N	2.254	2.143
N	-0.263	-0.292	N−Te	1.967	1.638
Te	0.255	-0.114	Ru−Cl_1	1.322	1.302
Cl_1	0.015	-0.029	Ru−Cl_2	1.321	1.283
Cl_2	0.014	-0.074	Ru−O_1	0.642	0.552
O_1	-0.127	-0.124	Ru−O_2	0.629	0.599
O_2	-0.137	-0.118	Ru−O_3	0.623	0.453
O_3	-0.139	-0.150	P_1−O_1	1.903	1.988
N−Te	-0.008	-0.406	P_2−O_2	1.895	1.951
P_1−O_1	0.194	0.202	P_3−O_3	1.903	2.048
P_2−O_2	0.181	0.197	—	—	—
P_3−O_3	0.185	0.171	—	—	—

P_1−O_1 is *trans* to Cl_1; P_2−O_2 is *trans* to Cl_2; P_3−O_3 is *trans* to N−X, X = O, S, Se, Te.

Table S2: Bond length (Å), Löwdin Bond Order ($b_{AB}^{Löwdin}$), vibrational frequency ($\nu_{\text{N-E}}$, cm^{-1}) and Hirshfeld charge for the diatomic chalcogenonitrosyl molecules.

	bond length		$b_{AB}^{Löwdin}$		$\nu_{\text{N-E}}$		Hirshfield	
	$(\text{N}-\text{E})^+$	$(\text{N}-\text{E})^0$	$(\text{N}-\text{E})^+$	$(\text{N}-\text{E})^0$	$(\text{N}-\text{E})^+$	$(\text{N}-\text{E})^0$	$(\text{N}-\text{E})^+$	$(\text{N}-\text{E})^0$
N≡O	1.070	1.158	3.602	3.034	2356	1880	1	0
N≡S	1.444	1.507	3.580	2.998	1429	1203	1	0
N≡Se	1.592	1.664	3.573	3.053	1132	959	1	0
N≡Te	1.807	1.876	3.425	2.749	947	807	1	0

Table S3: Hirshfeld charge for the compounds **1a**-**4b**.

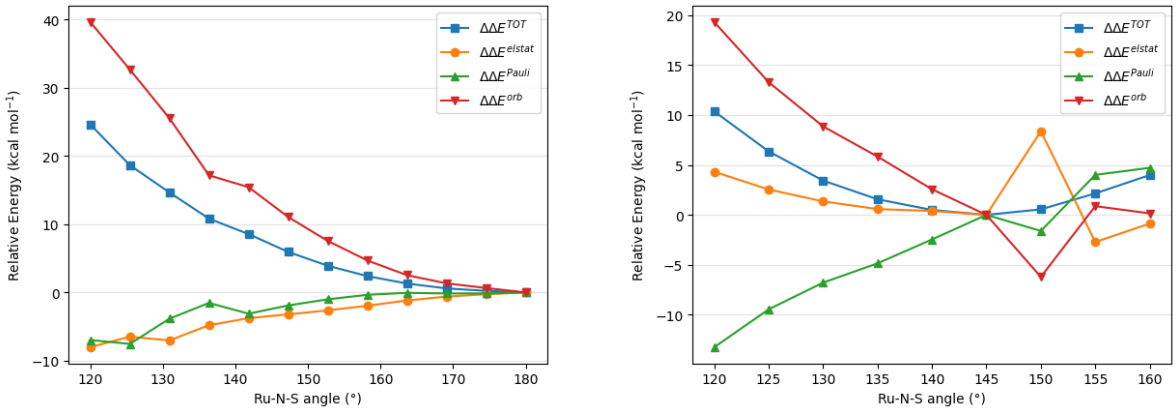
	1a	**1b**	**2a**	**2b**	**3a**	**3b**	**4a**	**4b**
Ru	0.47	0.35	0.50	0.38	0.50	0.41	0.51	0.42
N	0.04	-0.07	-0.10	-0.18	-0.12	-0.19	-0.17	-0.22
E	-0.02	-0.15	0.10	-0.14	0.11	-0.17	0.15	-0.18
Cl_1	-0.29	-0.36	-0.28	-0.34	-0.28	-0.33	-0.27	-0.32
Cl_2	-0.29	-0.36	-0.28	-0.35	-0.28	-0.35	-0.27	-0.34
O_1	-0.28	-0.27	-0.28	-0.27	-0.28	-0.27	-0.28	-0.27
O_2	-0.28	-0.27	-0.28	-0.27	-0.28	-0.26	-0.28	-0.26
O_3	-0.27	-0.29	-0.28	-0.28	-0.27	-0.29	-0.28	-0.29
$(NE)^{+/0}$	0.02	-0.22	0.00	-0.32	-0.01	-0.36	-0.02	-0.40
$[RuCl_2(L_{OEt})]^-$	-0.02	-0.78	0.00	-0.68	0.01	-0.64	0.02	-0.60

Table S4: CHELPG charge for the compounds **1a**-**4b**.

	1a	**1b**	**2a**	**2b**	**3a**	**3b**	**4a**	**4b**
Ru	-0.10	0.51	0.34	0.56	0.42	0.67	0.46	0.69
N	0.44	0.13	-0.05	-0.11	-0.14	-0.21	-0.17	-0.21
E	-0.17	-0.29	0.10	-0.20	0.14	-0.23	0.17	-0.27
Cl_1	-0.29	-0.45	-0.31	-0.43	-0.31	-0.41	-0.32	-0.41
Cl_2	-0.30	-0.45	-0.31	-0.43	-0.32	-0.46	-0.32	-0.46
O_1	-0.34	-0.46	-0.35	-0.35	-0.36	-0.45	-0.37	-0.44
O_2	-0.28	-0.45	-0.31	-0.34	-0.31	-0.33	-0.31	-0.25
O_3	-0.15	-0.38	-0.32	-0.42	-0.35	-0.45	-0.35	-0.45
$(NE)^{+/0}$	0.27	-0.16	0.05	-0.32	0.00	-0.45	0.00	-0.48
$[RuCl_2(L_{OEt})]^-$	-0.27	-0.84	-0.05	-0.68	0.00	-0.55	0.00	-0.52

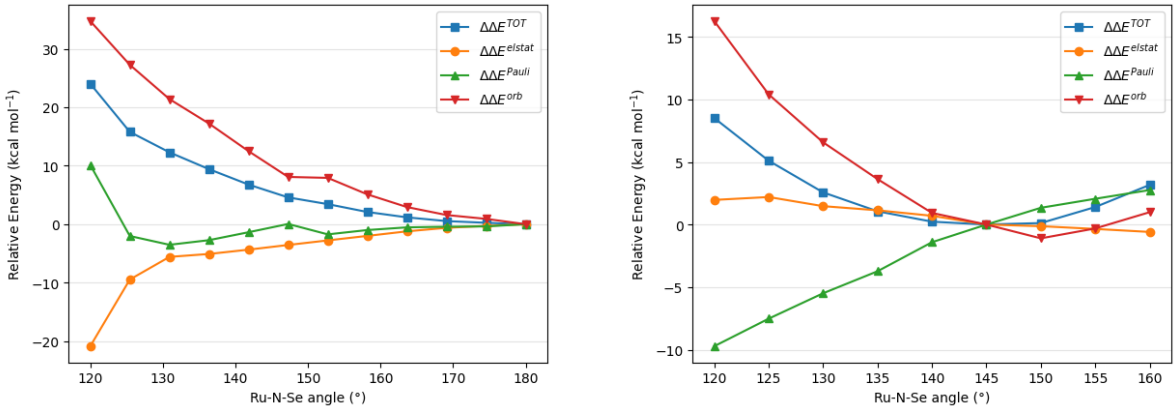
Table S5: Frontier Molecular Orbital Population Analysis, Löwdin Atomic charge. Energy in eV.

Complex	HOMO						LUMO					
	Ru	NE	Cl_1	Cl_2	L_{OEt}^-	Energy	Ru	NE	Cl_1	Cl_2	L_{OEt}^-	Energy
1a	0.56	0.00	0.17	0.18	0.08	-4.64	0.25	0.47	0.01	0.01	0.27	-2.91
2a	0.57	0.00	0.17	0.18	0.09	-4.60	0.32	0.60	0.01	0.01	0.05	-3.39
3a	0.56	0.00	0.17	0.18	0.09	-4.63	0.34	0.58	0.01	0.02	0.05	-3.40
4a	0.56	0.00	0.17	0.18	0.09	-4.65	0.35	0.57	0.02	0.02	0.05	-3.48
	SOMO						LUMO					
1b	0.48	0.39	0.03	0.03	0.08	-0.16	0.00	0.00	0.00	0.00	0.99	0.12
2b	0.38	0.49	0.02	0.02	0.09	-0.14	0.00	0.01	0.00	0.00	0.99	0.10
3b	0.41	0.48	0.02	0.02	0.07	-0.43	0.02	0.01	0.00	0.00	0.98	0.02
4b	0.40	0.51	0.02	0.02	0.05	-0.61	0.01	0.00	0.00	0.00	0.99	-0.04



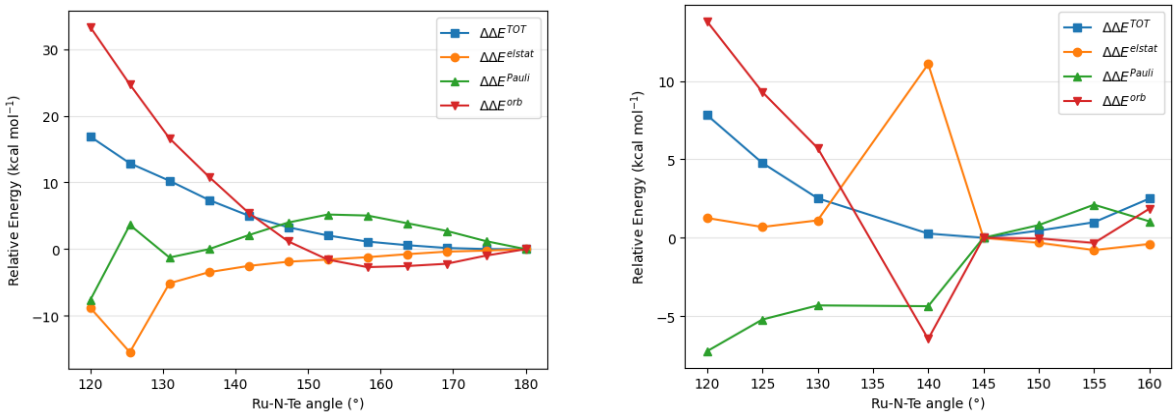
(a) GKS-EDA **2a**. (b) GKS-EDA **2b**.

Figure S3: Relative values of GKS-EDA components obtained by bending the angle Ru−N−S.



(a) GKS-EDA **3a**. (b) GKS-EDA **3b**.

Figure S4: Relative values of GKS-EDA components obtained by bending the angle Ru−N−Se.



(a) GKS-EDA **4a**.

(b) GKS-EDA **4b**.

Figure S5: Relative values of GKS-EDA components obtained by bending the angle Ru−N−Te.

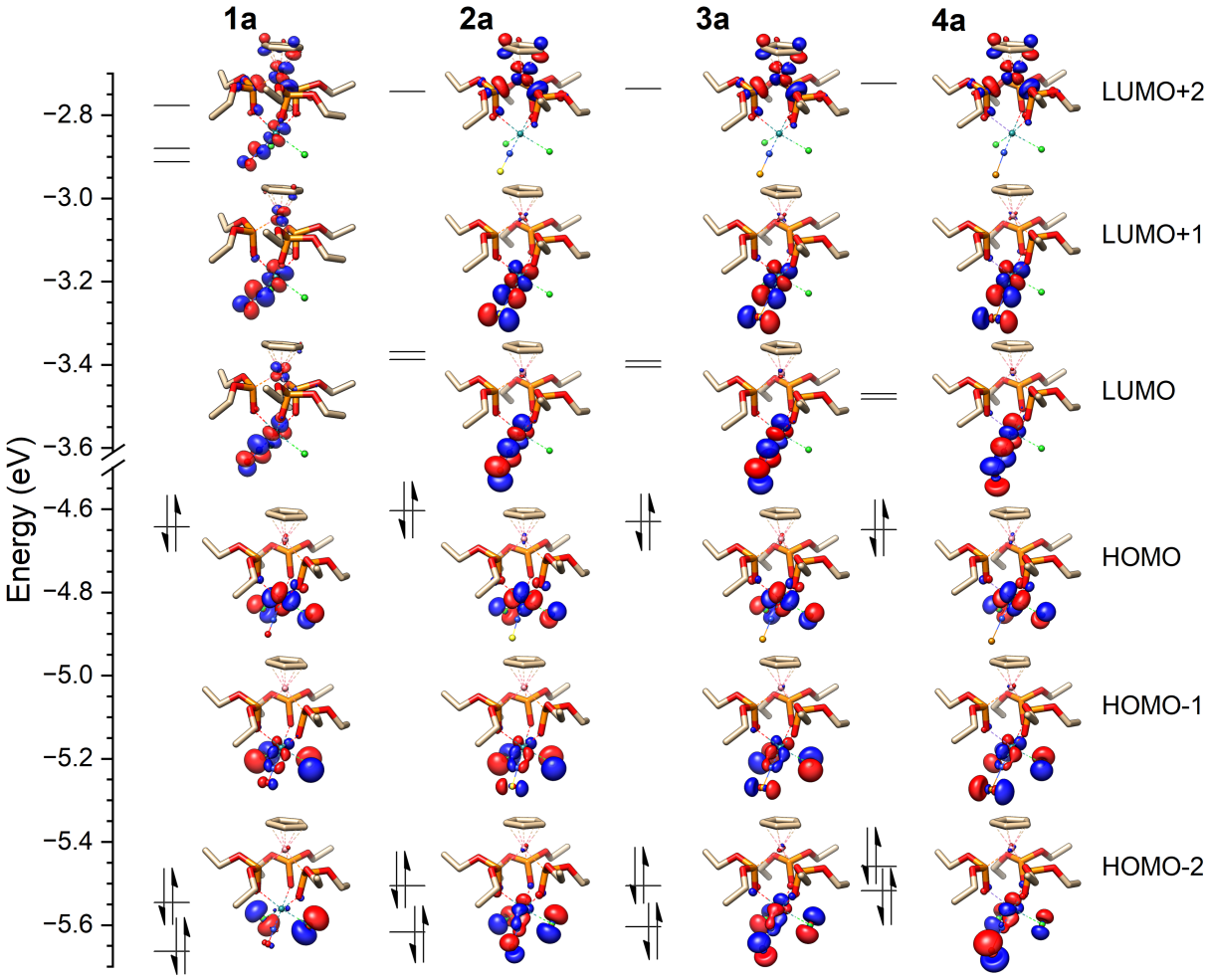


Figure S6: Frontier molecular orbitals and energies for the oxidized compounds. Isosurface value 0.06.

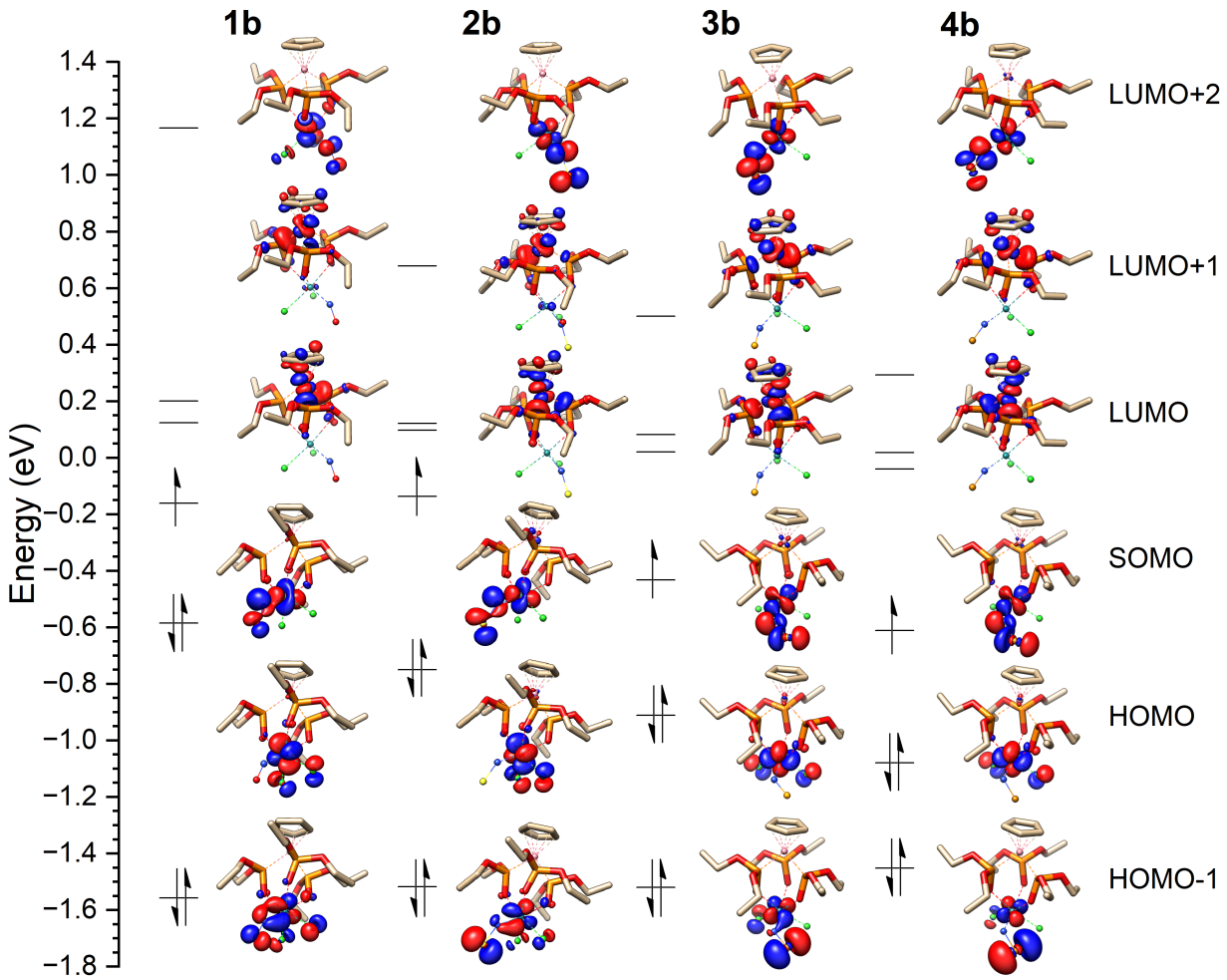


Figure S7: Frontier molecular orbitals and energies for the reduced compounds. Isosurface value 0.06.

Table S6: Cartesian coordinates for the optimized structure **1a**.

	x	y	z
N	11.908905000	12.876338000	2.819871000
O	11.468070000	13.087637000	1.765421000
Ru	12.566782000	12.562210000	4.373654000
Cl	11.885119000	14.624719000	5.234848000
Cl	10.617255000	11.503659000	5.114947000
P	14.594345000	11.388153000	6.680197000
O	14.077063000	9.997467000	7.325060000
O	14.437996000	13.383996000	3.822567000
O	13.367744000	12.205983000	6.219922000
O	13.352889000	10.679748000	3.846329000
C	14.272140000	12.462662000	9.072719000
H	13.495316000	13.129814000	8.671652000
H	13.790233000	11.539234000	9.427050000
C	12.794136000	9.385909000	6.980788000
H	12.455161000	9.745067000	6.000454000
H	13.006030000	8.309626000	6.918956000
C	11.760089000	9.701654000	8.039920000
H	11.529877000	10.774732000	8.040427000
H	10.828182000	9.164947000	7.809471000
H	12.102388000	9.392917000	9.038371000
C	13.728431000	7.776206000	3.670305000
O	14.740265000	8.608985000	4.314394000
H	12.737548000	8.193809000	3.898676000
H	13.881528000	7.817595000	2.580926000
C	13.887519000	6.368264000	4.200555000
H	13.748690000	6.340908000	5.289987000
H	13.133716000	5.712356000	3.741667000
C	13.830636000	10.484194000	0.566320000
Co	16.198342000	11.110506000	5.276420000
P	15.810779000	13.046500000	4.437261000
P	14.808583000	10.178564000	3.923158000
O	16.887727000	13.243737000	3.228648000
O	16.193570000	14.194470000	5.510272000
O	15.191384000	12.119384000	7.990470000
O	15.388639000	10.069130000	2.404918000
C	18.201054000	11.643584000	5.555855000
H	18.577319000	12.657804000	5.471392000
C	17.692581000	11.041396000	6.742513000
H	17.601178000	11.521009000	7.710306000
C	17.257775000	9.713539000	6.413510000
H	16.788226000	9.007008000	7.089929000
C	17.517341000	9.502484000	5.025137000
H	17.278620000	8.602490000	4.468839000
C	18.091324000	10.694387000	4.486160000
H	18.362776000	10.865294000	3.450592000
C	16.832843000	14.461125000	2.433850000
H	15.810601000	14.589068000	2.048050000
H	17.067311000	15.319096000	3.084490000
C	17.842027000	14.329596000	1.313282000
H	17.600708000	13.472487000	0.669829000
H	17.834149000	15.238168000	0.694046000
H	18.856745000	14.191942000	1.711401000
C	15.441046000	15.445513000	5.637606000
H	14.620807000	15.452695000	4.907992000
H	14.149626000	14.796272000	7.229128000
C	14.901539000	15.572229000	7.043238000
H	15.708563000	15.499341000	7.785368000
C	15.077591000	13.126609000	10.167286000
H	14.412523000	13.405255000	10.997361000
H	15.565888000	14.037254000	9.796290000
H	15.848767000	12.447661000	10.557109000
H	14.883027000	5.967266000	3.965407000
C	14.977237000	11.033197000	1.391842000
H	16.154841000	16.249193000	5.399316000
H	14.408631000	16.549029000	7.155564000
H	13.565711000	11.199268000	-0.226719000
H	14.110574000	9.532437000	0.092999000
H	12.944797000	10.321199000	1.193449000
H	15.873135000	11.203263000	0.778724000
H	14.706440000	11.982616000	1.873893000

Table S7: Cartesian coordinates for the optimized structure **2a**.

	x	y	z
N	11.959367000	12.895466000	2.783675000
S	11.454894000	13.207720000	1.377071000
Ru	12.559148000	12.573704000	4.363424000
Cl	11.868086000	14.617332000	5.226187000
Cl	10.616041000	11.521740000	5.084401000
P	14.598263000	11.388973000	6.690118000
O	14.081787000	9.991381000	7.324921000
O	14.432107000	13.394801000	3.838187000
O	13.376069000	12.207955000	6.233001000
O	13.349133000	10.694532000	3.845307000
C	14.289318000	12.446002000	9.091097000
H	13.509434000	13.112851000	8.695132000
H	13.810217000	11.521024000	9.445541000
C	12.789301000	9.399188000	6.982464000
H	12.462822000	9.751005000	5.995251000
H	12.982686000	8.318596000	6.934873000
C	11.754182000	9.744471000	8.031367000
H	11.544497000	10.821729000	8.021006000
H	10.813654000	9.223526000	7.799413000
H	12.084042000	9.438288000	9.034828000
C	13.723822000	7.789273000	3.669485000
O	14.733031000	8.621675000	4.316651000
H	12.732144000	8.209378000	3.890093000
H	13.883783000	7.826201000	2.580824000
C	13.876826000	6.382734000	4.205699000
H	13.732589000	6.360346000	5.294553000
H	13.123872000	5.726615000	3.745591000
C	13.856570000	10.417000000	0.543025000
Co	16.197819000	11.116471000	5.279508000
P	15.807173000	13.053211000	4.443360000
P	14.804212000	10.191700000	3.926538000
O	16.876718000	13.247813000	3.227263000
O	16.199139000	14.204961000	5.510263000
O	15.204660000	12.106835000	8.005370000
O	15.391173000	10.086449000	2.411205000
C	18.200334000	11.649105000	5.559798000
H	18.574344000	12.665071000	5.485727000
C	17.695845000	11.032835000	6.740878000
H	17.604876000	11.501965000	7.713865000
C	17.261250000	9.708544000	6.397912000
H	16.794382000	8.993715000	7.067496000
C	17.518779000	9.513138000	5.006615000
H	17.279760000	8.619279000	4.440551000
C	18.090134000	10.711367000	4.479934000
H	18.356672000	10.894985000	3.445275000
C	16.810848000	14.461761000	2.428400000
H	15.786013000	14.581376000	2.046784000
H	17.042728000	15.323872000	3.074596000
C	17.815730000	14.331874000	1.303621000
H	17.575052000	13.471810000	0.663775000
H	17.801105000	15.238731000	0.681864000
H	18.832911000	14.199743000	1.697454000
C	15.434956000	15.446953000	5.650986000
H	14.621377000	15.459535000	4.913982000
H	14.138994000	14.760968000	7.223800000
C	14.881334000	15.549735000	7.053260000
H	15.682619000	15.479215000	7.801862000
C	15.097050000	13.109957000	10.184192000
H	14.434234000	13.387917000	11.016374000
H	15.583508000	14.021174000	9.811879000
H	15.870144000	12.431649000	10.571443000
H	14.872718000	5.978684000	3.977253000
C	14.960141000	11.026316000	1.384762000
H	16.144960000	16.259133000	5.430911000
H	14.373366000	16.518031000	7.172432000
H	13.578897000	11.109178000	-0.266020000
H	14.186650000	9.471438000	0.089935000
H	12.964659000	10.229417000	1.154396000
H	15.859782000	11.231278000	0.787893000
H	14.636661000	11.965737000	1.853583000

Table S8: Cartesian coordinates for the optimized structure **3a**.

	x	y	z
N	11.977507000	12.915897000	2.783844000
Se	11.462218000	13.308938000	1.231038000
Ru	12.554777000	12.576778000	4.359026000
Cl	11.861190000	14.612076000	5.239221000
Cl	10.614327000	11.517616000	5.071679000
P	14.597078000	11.388985000	6.692684000
O	14.082414000	9.990866000	7.327630000
O	14.429405000	13.400886000	3.849773000
O	13.373247000	12.202890000	6.233708000
O	13.348454000	10.700695000	3.843531000
C	14.286442000	12.448651000	9.092000000
H	13.507111000	13.115474000	8.694882000
H	13.806616000	11.524018000	9.446408000
C	12.790422000	9.398815000	6.983383000
H	12.467290000	9.747584000	5.993953000
H	12.982964000	8.317912000	6.939939000
C	11.751950000	9.748784000	8.027532000
H	11.542664000	10.826063000	8.011682000
H	10.812096000	9.226835000	7.795149000
H	12.078662000	9.447191000	9.033408000
C	13.720254000	7.796965000	3.666763000
O	14.729751000	8.627293000	4.316105000
H	12.728567000	8.214935000	3.891311000
H	13.877821000	7.839354000	2.577946000
C	13.876000000	6.388021000	4.195795000
H	13.734215000	6.360120000	5.284851000
H	13.122796000	5.733238000	3.734187000
C	13.870834000	10.387051000	0.531924000
Co	16.196643000	11.119056000	5.281808000
P	15.806526000	13.056069000	4.447205000
P	14.803536000	10.197587000	3.926821000
O	16.870034000	13.246669000	3.225170000
O	16.205654000	14.209902000	5.509444000
O	15.202905000	12.108622000	8.007478000
O	15.393870000	10.093928000	2.413502000
C	18.198133000	11.651611000	5.568054000
H	18.571472000	12.668337000	5.500952000
C	17.692452000	11.027526000	6.744600000
H	17.599979000	11.490566000	7.720370000
C	17.259664000	9.705004000	6.392992000
H	16.792512000	8.985706000	7.057563000
C	17.519304000	9.518458000	5.000750000
H	17.282097000	8.627893000	4.428727000
C	18.090479000	10.720222000	4.482358000
H	18.358103000	10.910446000	3.449193000
C	16.796121000	14.455878000	2.419699000
H	15.769231000	14.569077000	2.041722000
H	17.027003000	15.322673000	3.060027000
C	17.797114000	14.323626000	1.291806000
H	17.557705000	13.458552000	0.658222000
H	17.775784000	15.226484000	0.664444000
H	18.816517000	14.198455000	1.682146000
C	15.439744000	15.450495000	5.653375000
H	14.627322000	15.464755000	4.915177000
H	14.141209000	14.759275000	7.221990000
C	14.883695000	15.548683000	7.055069000
H	15.683816000	15.475869000	7.804668000
C	15.093058000	13.112698000	10.185868000
H	14.429298000	13.391105000	11.017151000
H	15.580366000	14.023637000	9.814000000
H	15.865422000	12.434192000	10.574224000
H	14.871870000	5.986253000	3.963240000
C	14.954462000	11.022134000	1.380053000
H	16.149539000	16.263716000	5.436772000
H	14.375431000	16.516547000	7.176557000
H	13.589227000	11.067548000	-0.285581000
H	14.222033000	9.443542000	0.090401000
H	12.975341000	10.190683000	1.135398000
H	15.855409000	11.242826000	0.790875000
H	14.607386000	11.956645000	1.841924000

Table S9: Cartesian coordinates for the optimized structure **4a**.

	x	y	z
N	11.967727000	12.911820000	2.785301000
Te	11.394731000	13.352796000	1.032632000
Ru	12.535336000	12.582137000	4.359064000
Cl	11.848741000	14.612283000	5.246539000
Cl	10.602397000	11.527648000	5.087829000
P	14.593037000	11.392312000	6.698955000
O	14.080593000	9.994750000	7.339689000
O	14.411036000	13.403084000	3.856802000
O	13.369606000	12.205508000	6.241992000
O	13.328791000	10.704924000	3.846819000
C	14.298068000	12.453846000	9.099163000
H	13.518010000	13.121985000	8.705625000
H	13.818149000	11.530584000	9.457044000
C	12.786778000	9.405210000	6.998294000
H	12.462590000	9.753565000	6.009075000
H	12.976520000	8.323770000	6.955182000
C	11.751355000	9.758370000	8.044422000
H	11.545843000	10.836386000	8.029417000
H	10.809219000	9.239665000	7.813941000
H	12.079295000	9.455469000	9.049501000
C	13.693814000	7.801828000	3.672530000
O	14.705834000	8.629670000	4.321141000
H	12.703336000	8.221885000	3.898445000
H	13.850275000	7.844724000	2.583520000
C	13.847078000	6.392296000	4.200674000
H	13.706827000	6.364312000	5.289936000
H	13.091569000	5.739539000	3.739947000
C	13.994036000	10.359916000	0.435188000
Co	16.184129000	11.117834000	5.279836000
P	15.790869000	13.054409000	4.445538000
P	14.783245000	10.199485000	3.931140000
O	16.846126000	13.243527000	3.216183000
O	16.198591000	14.208167000	5.504913000
O	15.208074000	12.111126000	8.010349000
O	15.373175000	10.089805000	2.418561000
C	18.187306000	11.646568000	5.559751000
H	18.561615000	12.663087000	5.494709000
C	17.685650000	11.019056000	6.736139000
H	17.597772000	11.478897000	7.713844000
C	17.249327000	9.698490000	6.381587000
H	16.783448000	8.977629000	7.045341000
C	17.503522000	9.516365000	4.987680000
H	17.262427000	8.628257000	4.413461000
C	18.074569000	10.718828000	4.471317000
H	18.338117000	10.912295000	3.437711000
C	16.764461000	14.451347000	2.409157000
H	15.735527000	14.560123000	2.035582000
H	16.995213000	15.319920000	3.047091000
C	17.760778000	14.321088000	1.276946000
H	17.520070000	13.455998000	0.643815000
H	17.734976000	15.224083000	0.649949000
H	18.782150000	14.197477000	1.662626000
C	15.436194000	15.450278000	5.651767000
H	14.623420000	15.468220000	4.914024000
H	14.137933000	14.758343000	7.220125000
C	14.881037000	15.547356000	7.053918000
H	15.681455000	15.472400000	7.802974000
C	15.111698000	13.117644000	10.188043000
H	14.452964000	13.398873000	11.022378000
H	15.599186000	14.026903000	9.812237000
H	15.884586000	12.438025000	10.573418000
H	14.841609000	5.988164000	3.966485000
C	14.963006000	11.031304000	1.386247000
H	16.147936000	16.262096000	5.436244000
H	14.373944000	16.515622000	7.177159000
H	13.735011000	11.049229000	-0.382275000
H	14.436532000	9.453861000	-0.002799000
H	13.066886000	10.089349000	0.957483000
H	15.889914000	11.335794000	0.880478000
H	14.515915000	11.922035000	1.847858000

Table S10: Cartesian coordinates for the optimized structure **1b**.

	x	y	z
N	11.913319000	12.809031000	2.526581000
O	10.865031000	13.139641000	2.044691000
Ru	12.768573000	12.527182000	4.068367000
Cl	12.156317000	14.602468000	4.986566000
Cl	10.924296000	11.449126000	5.044067000
P	15.219052000	11.235217000	6.095287000
O	14.769812000	9.764080000	6.656729000
O	14.619910000	13.360504000	3.316471000
O	14.002689000	12.129843000	5.944461000
O	13.565610000	10.598552000	3.485465000
C	15.397160000	11.986828000	8.616791000
H	14.549578000	12.659742000	8.417025000
H	14.993950000	11.033437000	8.995311000
C	13.396129000	9.298002000	6.505417000
H	12.951040000	9.710058000	5.589630000
H	13.485695000	8.205676000	6.403648000
C	12.551990000	9.681598000	7.704044000
H	12.416114000	10.770125000	7.732361000
H	11.552526000	9.232838000	7.602942000
H	13.005818000	9.330779000	8.644360000
C	13.973504000	7.762844000	3.076077000
O	15.093276000	8.565102000	3.526843000
H	13.038756000	8.229129000	3.420134000
H	13.965179000	7.749068000	1.973378000
C	14.147905000	6.369680000	3.646387000
H	14.164821000	6.404061000	4.744684000
H	13.311827000	5.726967000	3.332087000
C	13.411615000	10.585094000	0.218857000
Co	16.606546000	11.060620000	4.435084000
P	16.038863000	13.026718000	3.765538000
P	15.017092000	10.180860000	3.273441000
O	17.004256000	13.336793000	2.464033000
O	16.538549000	14.137549000	4.848997000
O	16.108173000	11.737491000	7.381479000
O	15.352139000	10.212347000	1.667406000
C	18.625140000	11.623706000	4.363008000
H	18.953039000	12.648300000	4.221852000
C	18.344845000	11.004344000	5.614816000
H	18.399011000	11.479399000	6.587243000
C	17.877853000	9.672987000	5.353069000
H	17.538497000	8.956027000	6.093842000
C	17.891524000	9.477362000	3.938280000
H	17.556921000	8.583593000	3.423073000
C	18.347033000	10.681998000	3.319002000
H	18.416126000	10.871496000	2.253661000
C	16.743834000	14.543964000	1.714387000
H	15.674375000	14.587834000	1.458716000
H	16.979084000	15.419933000	2.343678000
C	17.613395000	14.516192000	0.472323000
H	17.369960000	13.642538000	-0.148691000
H	17.447654000	15.424238000	-0.126783000
H	18.679116000	14.464947000	0.738547000
C	15.696636000	15.273280000	5.219157000
H	14.773030000	15.261078000	4.623098000
H	14.682110000	14.361843000	6.874604000
C	15.354733000	15.208598000	6.692183000
H	16.261076000	15.110674000	7.308014000
C	16.374657000	12.600635000	9.599052000
H	15.869610000	12.805250000	10.555148000
H	16.772795000	13.547220000	9.208422000
H	17.217391000	11.920367000	9.790428000
H	15.086566000	5.913617000	3.299469000
C	14.667699000	11.183237000	0.822338000
H	16.285986000	16.173032000	4.975020000
H	14.822884000	16.127438000	6.981735000
H	12.947747000	11.310960000	-0.466368000
H	13.639606000	9.666771000	-0.343869000
H	12.684450000	10.359392000	1.009086000
H	15.402227000	11.453071000	0.048502000
H	14.423018000	12.082377000	1.404383000

Table S11: Cartesian coordinates for the optimized structure **2b**.

	x	y	z
N	12.028345000	12.756827000	2.568052000
S	10.859366000	13.155556000	1.594364000
Ru	12.582408000	12.576534000	4.249872000
Cl	11.865198000	14.706425000	4.891430000
Cl	10.581087000	11.598199000	4.956850000
P	14.630419000	11.416570000	6.678686000
O	14.083472000	9.994789000	7.276296000
O	14.535864000	13.342451000	3.734977000
O	13.455604000	12.292109000	6.269149000
O	13.387548000	10.606254000	3.911439000
C	14.383787000	12.408950000	9.109222000
H	13.603338000	13.069009000	8.701680000
H	13.894879000	11.499976000	9.496169000
C	12.755427000	9.501609000	6.927856000
H	12.466114000	9.855994000	5.929620000
H	12.863339000	8.406420000	6.904355000
C	11.726381000	9.940759000	7.950134000
H	11.587143000	11.028145000	7.899081000
H	10.757175000	9.477722000	7.711802000
H	12.020466000	9.644419000	8.969338000
C	13.878944000	7.751584000	3.641542000
O	14.895655000	8.587800000	4.248105000
H	12.900885000	8.243247000	3.748597000
H	14.098129000	7.649509000	2.565646000
C	13.908112000	6.408430000	4.342475000
H	13.688147000	6.527859000	5.412618000
H	13.150954000	5.739919000	3.905774000
C	13.664646000	10.391953000	0.675953000
Co	16.259827000	11.099583000	5.278779000
P	15.859901000	13.035023000	4.430562000
P	14.856878000	10.190239000	3.917934000
O	17.028551000	13.288811000	3.297037000
O	16.170259000	14.198633000	5.530978000
O	15.292045000	12.036368000	8.045127000
O	15.418583000	10.174302000	2.380696000
C	18.211786000	11.596119000	5.844970000
H	18.545026000	12.615239000	6.013829000
C	17.641439000	10.729418000	6.822062000
H	17.441687000	10.987073000	7.855856000
C	17.280205000	9.504085000	6.176483000
H	16.771347000	8.662431000	6.633779000
C	17.664375000	9.610523000	4.799825000
H	17.498011000	8.856169000	4.038014000
C	18.239585000	10.894441000	4.590410000
H	18.572316000	11.301545000	3.642637000
C	16.919252000	14.476222000	2.478426000
H	15.884270000	14.572664000	2.117357000
H	17.152216000	15.361123000	3.095783000
C	17.897813000	14.340135000	1.328410000
H	17.651971000	13.460843000	0.716684000
H	17.854047000	15.232565000	0.686017000
H	18.927588000	14.228624000	1.698030000
C	15.331586000	15.390743000	5.628998000
H	14.541226000	15.350926000	4.866536000
H	14.004188000	14.648760000	7.141810000
C	14.712745000	15.474672000	7.006879000
H	15.482901000	15.446254000	7.792150000
C	15.191680000	13.104169000	10.186315000
H	14.532378000	13.409690000	11.012740000
H	15.680439000	14.001450000	9.782735000
H	15.967128000	12.436883000	10.590227000
H	14.893203000	5.929710000	4.242502000
C	14.824213000	11.062991000	1.384895000
H	15.997928000	16.246628000	5.427919000
H	14.148652000	16.415388000	7.094543000
H	13.274923000	11.060823000	-0.106142000
H	13.976990000	9.444014000	0.211123000
H	12.847276000	10.205624000	1.383393000
H	15.647908000	11.292402000	0.692292000
H	14.494218000	11.994109000	1.864481000

Table S12: Cartesian coordinates for the optimized structure **3b**.

	x	y	z
N	12.130982000	12.865051000	2.567182000
Se	12.487286000	14.024389000	1.291696000
Ru	12.542037000	12.598858000	4.261562000
Cl	11.841674000	14.690209000	5.011038000
Cl	10.562098000	11.549270000	4.959624000
P	14.600900000	11.374252000	6.690858000
O	14.077981000	9.932886000	7.263369000
O	14.448355000	13.390774000	3.831696000
O	13.407731000	12.229189000	6.301848000
O	13.388541000	10.647095000	3.869028000
C	14.354287000	12.322649000	9.136313000
H	13.566895000	12.982870000	8.742399000
H	13.875329000	11.402418000	9.508516000
C	12.751762000	9.440179000	6.908949000
H	12.452779000	9.820617000	5.922811000
H	12.866525000	8.347063000	6.854954000
C	11.724356000	9.845768000	7.946641000
H	11.579408000	10.933354000	7.924675000
H	10.756913000	9.383257000	7.700173000
H	12.024282000	9.524706000	8.956550000
C	13.809343000	7.775604000	3.689738000
O	14.828758000	8.598553000	4.312488000
H	12.832027000	8.265147000	3.811996000
H	14.023865000	7.700043000	2.610940000
C	13.842807000	6.415985000	4.357464000
H	13.631505000	6.508072000	5.431992000
H	13.081169000	5.759919000	3.909953000
C	13.797845000	10.451281000	0.637205000
Co	16.232505000	11.126443000	5.289214000
P	15.802526000	13.060363000	4.452593000
P	14.842248000	10.189075000	3.933453000
O	16.901869000	13.289526000	3.254540000
O	16.180000000	14.220387000	5.533917000
O	15.262683000	11.977416000	8.062525000
O	15.447014000	10.093987000	2.417312000
C	18.233828000	11.690220000	5.559285000
H	18.580820000	12.715227000	5.477337000
C	17.747939000	11.067361000	6.744409000
H	17.642212000	11.539452000	7.714178000
C	17.330511000	9.736583000	6.405996000
H	16.869100000	9.019559000	7.077175000
C	17.581089000	9.543591000	5.012612000
H	17.340560000	8.650000000	4.446761000
C	18.132153000	10.749230000	4.481163000
H	18.374924000	10.940956000	3.442075000
C	16.698300000	14.413178000	2.358362000
H	15.646956000	14.430220000	2.030502000
H	16.902176000	15.348773000	2.907239000
C	17.645742000	14.250141000	1.187471000
H	17.428251000	13.321435000	0.641509000
H	17.527473000	15.093424000	0.490636000
H	18.692795000	14.219523000	1.523009000
C	15.343742000	15.409754000	5.686902000
H	14.552693000	15.405635000	4.924313000
H	14.028881000	14.597513000	7.175193000
C	14.728452000	15.435302000	7.068825000
H	15.501314000	15.385811000	7.850330000
C	15.159975000	13.006175000	10.222451000
H	14.501417000	13.288211000	11.057659000
H	15.636223000	13.916811000	9.833984000
H	15.944761000	12.339821000	10.609453000
H	14.826289000	5.938664000	4.237632000
C	14.969439000	11.030288000	1.403841000
H	16.014374000	16.268857000	5.520664000
H	14.154587000	16.365896000	7.193432000
H	13.489329000	11.162084000	-0.143915000
H	14.065522000	9.491461000	0.169195000
H	12.940491000	10.310200000	1.307626000
H	15.838000000	11.205610000	0.751999000
H	14.687933000	11.983260000	1.871050000

Table S13: Cartesian coordinates for the optimized structure **4b**.

	x	y	z
N	12.124447000	12.847723000	2.566525000
Te	12.503561000	14.210677000	1.163145000
Ru	12.531429000	12.595132000	4.247466000
Cl	11.824552000	14.674271000	5.004154000
Cl	10.561628000	11.543269000	4.954122000
P	14.598396000	11.374139000	6.687093000
O	14.080108000	9.932418000	7.262398000
O	14.438663000	13.391493000	3.831038000
O	13.402381000	12.222894000	6.293893000
O	13.384750000	10.646395000	3.862928000
C	14.349688000	12.329422000	9.129744000
H	13.562213000	12.988912000	8.734935000
H	13.871260000	11.409262000	9.502688000
C	12.755495000	9.434771000	6.909117000
H	12.456620000	9.811109000	5.921429000
H	12.873315000	8.341898000	6.858906000
C	11.726574000	9.841005000	7.945106000
H	11.579049000	10.928177000	7.920557000
H	10.760375000	9.375138000	7.699934000
H	12.026903000	9.523374000	8.955888000
C	13.808509000	7.773132000	3.689482000
O	14.824015000	8.599751000	4.314728000
H	12.829601000	8.260313000	3.808273000
H	14.026576000	7.697419000	2.611513000
C	13.843923000	6.414359000	4.358615000
H	13.628725000	6.506415000	5.432351000
H	13.085984000	5.755405000	3.909149000
C	13.796997000	10.424920000	0.630486000
Co	16.228484000	11.128109000	5.284094000
P	15.796489000	13.061043000	4.446064000
P	14.839004000	10.187775000	3.929176000
O	16.891874000	13.285861000	3.246877000
O	16.173736000	14.221918000	5.525525000
O	15.258453000	11.983191000	8.056139000
O	15.445502000	10.089959000	2.415991000
C	18.227028000	11.695767000	5.554007000
H	18.572520000	12.721379000	5.473399000
C	17.742929000	11.070364000	6.738597000
H	17.636888000	11.540974000	7.709048000
C	17.327479000	9.739447000	6.398485000
H	16.867625000	9.020585000	7.068742000
C	17.578359000	9.548824000	5.004674000
H	17.340437000	8.655160000	4.437810000
C	18.127428000	10.755820000	4.474611000
H	18.369105000	10.949586000	3.435684000
C	16.702905000	14.420304000	2.359259000
H	15.649868000	14.458484000	2.036942000
H	16.927995000	15.346933000	2.914778000
C	17.638418000	14.248517000	1.180635000
H	17.397399000	13.330216000	0.627121000
H	17.530877000	15.100537000	0.492855000
H	18.687329000	14.193999000	1.507346000
C	15.338015000	15.412437000	5.675394000
H	14.555269000	15.413239000	4.904456000
H	14.009756000	14.595360000	7.149559000
C	14.709723000	15.433844000	7.051591000
H	15.475677000	15.382387000	7.839700000
C	15.155348000	13.014211000	10.214950000
H	14.497065000	13.296946000	11.050104000
H	15.631275000	13.924629000	9.825593000
H	15.940305000	12.348375000	10.602402000
H	14.829278000	5.940130000	4.242195000
C	14.963683000	11.016646000	1.394390000
H	16.012467000	16.270093000	5.518847000
H	14.134605000	16.363914000	7.173902000
H	13.487031000	11.126754000	-0.158189000
H	14.070728000	9.462018000	0.172404000
H	12.938198000	10.286550000	1.299719000
H	15.832318000	11.192459000	0.743187000
H	14.676346000	11.971701000	1.853930000