# Supplementary information for

# Bimetallic Ru─Cu Tellurido Complexes: Controlled Synthesis and Electrochemical Studies of Copper Halide-$TeRu_5$ and $Te_2Ru_4$ Clusters

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**Table S1.** Cyclic Voltammetry of $[PPh_4]_2$[**1**], $[PPh_4]_2$[**2a**], $[PPh_4]_2$[**2b**], $[PPh_4]_2$[**2c**], $[PPh_4]_2$[**3a**], $[PPh_4]_2$[**3b**], $[PPh_4]_2$[**5a**], $[PPh_4]_2$[**5b**], and $[PPh_4]_2$[**5c**].

| Compound | Oxidation Process | Reduction Process | | | | |
|---|---|---|---|---|---|---|
| | $E_p^{ox}$/V[a], | $E_p^{ox}$/V[a] | | $E_p^{red}$ /V[b] | | |
| $[PPh_4]_2$[**1**] | 0.075 | | | ─1.257 | ─1.402 | ─1.910 |
| $[PPh_4]_2$[**2a**] | 0.117 | ─0.291 | ─0.680 | ─1.138 | ─1.458 | ─1.837 |
| $[PPh_4]_2$[**2b**] | ~ 0.169[c] | ─0.230 | ─0.597 | ─1.193 | ─1.402 | ─1.817 |
| $[PPh_4]_2$[**2c**] | 0.152 | ─0.246 | ─0.646 | -[c] | -[c] | ─1.811 |
| $[PPh_4]_2$[**3a**] | 0.238 | ─0.129 | ─0.467 | ─1.055 | -[c] | ─1.720 |
| $[PPh_4]_2$[**3b**] | 0.188 | ─0.179 | ─0.604 | ─1.174 | ─1.262 | ─1.828 |
| $[PPh_4]_2$[**5a**] | 0.203 | ─0.255 | ─0.617 | ─1.223 | ─1.455 | ─1.861 |
| $[PPh_4]_2$[**5b**] | 0.191 | ─0.303 | ─0.760 | -[c] | ─1.485 | ─1.864 |
| $[PPh_4]_2$[**5c**] | 0.198 | ─0.279 | ─0.683 | ─1.151 | ─1.396 | ─1.783 |

[a] $E_p^{ox}$ = oxidative peak potential. [b] $E_p^{red}$ = reductive peak potential. [c] Difficult to determine.

**Table S2.** Differential Pulse Voltammetry of $[PPh_4]_2$[**1**], $[PPh_4]_2$[**2a**], $[PPh_4]_2$[**2b**], $[PPh_4]_2$[**2c**], $[PPh_4]_2$[**3a**], $[PPh_4]_2$[**3b**], $[PPh_4]_2$[**5a**], $[PPh_4]_2$[**5b**], and $[PPh_4]_2$[**5c**].

| Compound | Oxidation Process | Reduction Process | | | |
|---|---|---|---|---|---|
| | $E_p^{red}$/V[a] | $E_p^{red}$/V[b] | | $E_p^{red}$/V[a] | |
| $[PPh_4]_2$[**1**] | 0.090 | | −1.178 | −1.474 | −1.798 |
| $[PPh_4]_2$[**2a**] | 0.134 | −0.866 | −1.086 | −1.326 | −1.770 |
| $[PPh_4]_2$[**2b**] | 0.139 | −0.577 | −1.141 | −1.405 | −1.781 |
| $[PPh_4]_2$[**2c**] | 0.132 | −0.632 | −1.184 | −1.428 | −1.824 |
| $[PPh_4]_2$[**3a**] | 0.180 | −0.540 | −1.124 | −1.396 | −1.776 |
| $[PPh_4]_2$[**3b**] | 0.202 | −0.618 | −1.134 | −1.394 | −1.778 |
| $[PPh_4]_2$[**5a**] | 0.200 | −0.870 | −1.146 | −1.426 | −1.770 |
| $[PPh_4]_2$[**5b**] | 0.166 | −0.718 | −1.222 | −1.458 | −1.826 |
| $[PPh_4]_2$[**5c**] | 0.162 | −0.636 | −1.116 | −1.356 | −1.748 |

[a] $E_p^{red}$ = The reductive peak potential of Ru atoms. [b] The reductive peak potential of Cu atom (desorption).

**Table S3.** Selected Bond Distances (Å) and Bond Angles (deg) for $[PPh_4]_2$[**1**]·$CH_2Cl_2$, $[PPh_4]_2$[**2a**], $[PPh_4]_2$[**2b**], $[PPh_4]_2$[**2c**], $[PPh_4]_2$[**3b**], $[PPh_4]_2$[**4b**], and $[PPh_4]_2$[**5c**].

| $[PPh_4]_2$[**1**]·$CH_2Cl_2$ | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.6650(7) | Ru(1)─Ru(5) | 2.8427(7) |
| Te(1)─Ru(2) | 2.7229(7) | Ru(2)─Ru(3) | 2.8155(7) |
| Te(1)─Ru(3) | 2.7481(7) | Ru(2)─Ru(5) | 2.8693(7) |
| Te(1)─Ru(4) | 2.6858(7) | Ru(3)─Ru(4) | 2.8456(7) |
| Ru(1)─Ru(2) | 2.8772(7) | Ru(3)─Ru(5) | 2.8815(7) |
| Ru(1)─Ru(4) | 2.8990(7) | Ru(4)─Ru(5) | 2.8412(8) |
| | | | |
| Ru(1)─Ru(2)─Ru(3) | 90.72(2) | Ru(2)─Ru(1)─Ru(4) | 88.65(2) |
| Ru(1)─Ru(4)─Ru(3) | 89.68(2) | Ru(2)─Ru(3)─Ru(4) | 90.95(2) |

| $[PPh_4]_2$[**2a**] | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.6764(4) | Ru(2)─Ru(5) | 2.9102(5) |
| Te(1)─Ru(2) | 2.7021(5) | Ru(3)─Ru(4) | 2.8348(5) |
| Te(1)─Ru(3) | 2.7463(4) | Ru(3)─Ru(5) | 2.8554(5) |
| Te(1)─Ru(4) | 2.6799(4) | Ru(4)─Ru(5) | 2.8686(5) |
| Ru(1)─Ru(2) | 2.8360(5) | Ru(1)─Cu(1) | 2.6284(6) |
| Ru(1)─Ru(4) | 3.0364(5) | Ru(4)─Cu(1) | 2.6229(6) |
| Ru(1)─Ru(5) | 2.8818(5) | Ru(5)─Cu(1) | 2.7893(7) |
| Ru(2)─Ru(3) | 2.8209(5) | Cu(1)─Cl(1) | 2.189(1) |
| | | | |
| Ru(1)─Ru(2)─Ru(3) | 92.18(1) | Cl(1)─Cu(1)─Ru(4) | 139.84(4) |
| Ru(1)─Ru(4)─Ru(3) | 87.85(1) | Cl(1)─Cu(1)─Ru(5) | 146.43(5) |
| Ru(2)─Ru(1)─Ru(4) | 87.79(1) | Ru(1)─Cu(1)─Ru(4) | 70.65(2) |
| Ru(2)─Ru(3)─Ru(4) | 92.16(1) | Ru(1)─Cu(1)─Ru(5) | 64.19(2) |
| Cl(1)─Cu(1)─Ru(1) | 136.48(5) | Ru(4)─Cu(1)─Ru(5) | 63.93(2) |

| $[PPh_4]_2$[**2b**] | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.6761(7) | Ru(2)─Ru(5) | 2.9085(7) |
| Te(1)─Ru(2) | 2.6982(8) | Ru(3)─Ru(4) | 2.8332(8) |
| Te(1)─Ru(3) | 2.7475(7) | Ru(3)─Ru(5) | 2.8545(8) |
| Te(1)─Ru(4) | 2.6786(6) | Ru(4)─Ru(5) | 2.8740(8) |
| Ru(1)─Ru(2) | 2.8347(8) | Ru(1)─Cu(1) | 2.6277(9) |
| Ru(1)─Ru(4) | 3.0349(7) | Ru(4)─Cu(1) | 2.621(1) |

| | | | |
|---|---|---|---|
| Ru(1)─Ru(5) | 2.8799(8) | Ru(5)─Cu(1) | 2.761(1) |
| Ru(2)─Ru(3) | 2.8200(8) | Br(1)─Cu(1) | 2.313(1) |
| | | | |
| Ru(1)─Ru(2)─Ru(3) | 92.17(2) | Ru(1)─Cu(1)─Ru(5) | 64.56(2) |
| Ru(1)─Ru(4)─Ru(3) | 87.86(2) | Ru(4)─Cu(1)─Ru(5) | 64.50(3) |
| Ru(2)─Ru(1)─Ru(4) | 87.78(2) | Br(1)─Cu(1)─Ru(1) | 136.74(4) |
| Ru(2)─Ru(3)─Ru(4) | 92.15(2) | Br(1)─Cu(1)─Ru(4) | 139.47(4) |
| Ru(1)─Cu(1)─Ru(4) | 70.65(3) | Br(1)─Cu(1)─Ru(5) | 145.93(5) |

| $[PPh_4]_2$[**2c**] | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.695(1) | Ru(2)─Ru(5) | 2.848(1) |
| Te(1)─Ru(2) | 2.746(2) | Ru(3)─Ru(4) | 2.850(2) |
| Te(1)─Ru(3) | 2.700(1) | Ru(3)─Ru(5) | 2.860(2) |
| Te(1)─Ru(4) | 2.690(1) | Ru(4)─Ru(5) | 2.889(2) |
| Ru(1)─Ru(2) | 2.810(2) | Ru(1)─Cu(1) | 2.667(2) |
| Ru(1)─Ru(4) | 2.997(2) | Ru(4)─Cu(1) | 2.658(2) |
| Ru(1)─Ru(5) | 2.905(2) | Ru(5)─Cu(1) | 2.693(2) |
| Ru(2)─Ru(3) | 2.839(2) | I(1)─Cu(1) | 2.486(2) |
| | | | |
| Ru(1)─Ru(2)─Ru(3) | 91.82(5) | Ru(1)─Cu(1)─Ru(5) | 65.65(5) |
| Ru(1)─Ru(4)─Ru(3) | 87.84(4) | Ru(4)─Cu(1)─Ru(5) | 65.35(5) |
| Ru(2)─Ru(1)─Ru(4) | 88.95(4) | I(1)─Cu(1)─Ru(1) | 140.53(8) |
| Ru(2)─Ru(3)─Ru(4) | 91.37(4) | I(1)─Cu(1)─Ru(4) | 144.17(8) |
| Ru(1)─Cu(1)─Ru(4) | 68.51(5) | I(1)─Cu(1)─Ru(5) | 136.75(8) |

| $[PPh_4]_2$[**3b**] | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.677(3) | Ru(4)─Ru(5) | 2.827(2) |
| Te(1)─Ru(2) | 2.675(2) | Cu(1)─Ru(1) | 2.636(2) |
| Te(1)─Ru(3) | 2.735(1) | Cu(1)─Ru(2) | 2.617(2) |
| Te(1)─Ru(4) | 2.715(2) | Cu(2a)─Ru(1) | 2.651(2) |
| Ru(1)─Ru(2) | 3.071(2) | Cu(2a)─Ru(2) | 2.633(3) |
| Ru(1)─Ru(4) | 2.809(2) | Cu(2a)─Ru(5) | 2.682(2) |
| Ru(1)─Ru(5) | 2.908(1) | Cu(1)─Cu(2) | 2.773(2) |
| Ru(2)─Ru(3) | 2.806(2) | Cu(1)─Cu(2a) | 2.598(3) |
| Ru(2)─Ru(5) | 2.929(2) | Br(1)─Cu(1) | 2.324(2) |
| Ru(3)─Ru(4) | 2.818(2) | Br(1)─Cu(2) | 2.331(3) |
| Ru(3)─Ru(5) | 2.800(4) | | |

| | | | |
|---|---|---|---|
| Ru(1)─Ru(2)─Ru(3) | 87.24(5) | Ru(2a)─Cu(2)─Ru(5a) | 66.88(6) |
| Ru(1)─Ru(4)─Ru(3) | 92.31(5) | Cu(1)─Cu(2)─Cu(1a) | 72.05(8) |
| Ru(2)─Ru(1)─Ru(4) | 87.59(5) | Cu(2)─Cu(1)─Cu(2a) | 107.95(8) |
| Ru(2)─Ru(3)─Ru(4) | 92.84(5) | Cu(1)─Ru(1)─Cu(2a) | 58.87(5) |
| Ru(1)─Cu(1)─Ru(2) | 71.54(5) | Cu(1)─Ru(2)─Cu(2a) | 59.33(6) |
| Ru(1a)─Cu(2)─Ru(2a) | 71.06(7) | Cu(1)─Br(1)─Cu(2) | 73.12(7) |
| Ru(1a)─Cu(2)─Ru(5a) | 66.08(4) | | |

$[PPh_4]_2$[**4b**]

| | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.674(1) | Ru(3)─Ru(5) | 2.883(2) |
| Te(1)─Ru(2) | 2.703(1) | Ru(4)─Ru(5) | 2.904(1) |
| Te(1)─Ru(3) | 2.744(1) | Ru(1)─Cu(1) | 2.671(2) |
| Te(1)─Ru(4) | 2.691(1) | Ru(1)─Cu(2) | 2.671(2) |
| Ru(1)─Ru(2) | 2.984(1) | Ru(2)─Cu(2) | 2.655(2) |
| Ru(1)─Ru(4) | 3.016(1) | Ru(4)─Cu(1) | 2.627(2) |
| Ru(1)─Ru(5) | 2.909(1) | Ru(5)─Cu(1) | 2.736(2) |
| Ru(2)─Ru(3) | 2.807(1) | Ru(5)─Cu(2) | 2.665(2) |
| Ru(2)─Ru(5) | 2.899(1) | Br(1)─Cu(1) | 2.299(2) |
| Ru(3)─Ru(4) | 2.803(1) | Br(2)─Cu(2) | 2.273(3) |

| | | | |
|---|---|---|---|
| Ru(1)─Ru(2)─Ru(3) | 90.46(3) | Ru(2)─Cu(2)─Ru(5) | 66.04(5) |
| Ru(1)─Ru(4)─Ru(3) | 89.89(3) | Cu(1)─Ru(1)─Cu(2) | 95.58(6) |
| Ru(2)─Ru(3)─Ru(4) | 93.66(4) | Cu(1)─Ru(5)─Cu(2) | 94.20(6) |
| Ru(2)─Ru(1)─Ru(4) | 85.99(3) | Br(1)─Cu(1)─Ru(1) | 143.47(8) |
| Ru(1)─Cu(1)─Ru(4) | 69.39(4) | Br(1)─Cu(1)─Ru(4) | 138.33(8) |
| Ru(1)─Cu(1)─Ru(5) | 65.07(4) | Br(1)─Cu(1)─Ru(5) | 139.75(8) |
| Ru(4)─Cu(1)─Ru(5) | 65.52(4) | Br(2)─Cu(2)─Ru(1) | 132.7(1) |
| Ru(1)─Cu(2)─Ru(2) | 68.15(5) | Br(2)─Cu(2)─Ru(2) | 138.0(1) |
| Ru(1)─Cu(2)─Ru(5) | 66.06(5) | Br(2)─Cu(2)─Ru(5) | 150.0(1) |

$[PPh_4]_2$[**5c**]

| | | | |
|---|---|---|---|
| Te(1)─Ru(1) | 2.7372(8) | Ru(1)─Ru(2a) | 2.8023(9) |
| Te(1)─Ru(2) | 2.7421(8) | Ru(1)─Cu(1) | 2.614(1) |
| Te(1)─Ru(1a) | 2.7474(8) | Ru(2)─Cu(1) | 2.601(1) |
| Te(1)─Ru(2a) | 2.7395(9) | I(1)─Cu(1) | 2.441(1) |
| Ru(1)─Ru(2) | 3.0121(9) | | |

| | | | |
|---|---|---|---|
| Ru(1a)─Ru(2)─Ru(1) | 90.06(2) | I(1)─Cu(1)─Ru(1) | 140.95(5) |
| Ru(2)─Ru(1)─Ru(2a) | 89.94(2) | I(1)─Cu(1)─Ru(2) | 148.49(5) |
| Ru(1)─Cu(1)─Ru(2) | 70.56(3) | | |

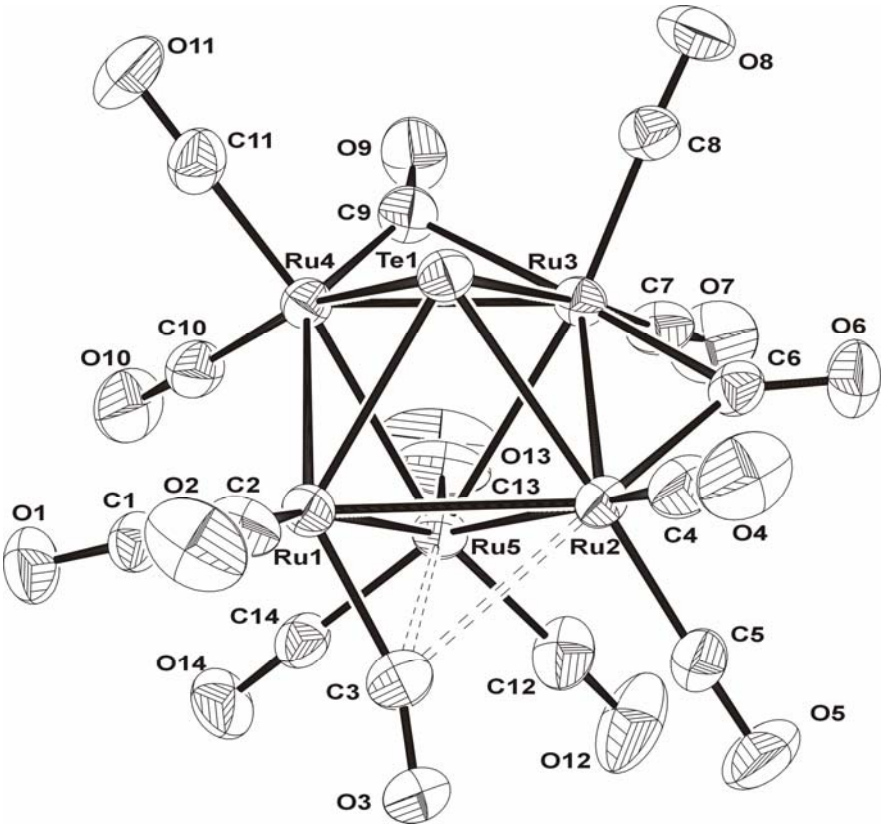


**Figure S1.** ORTEP diagram (30% thermal ellipsoids) showing the structure and atom labeling for the anion **1**.

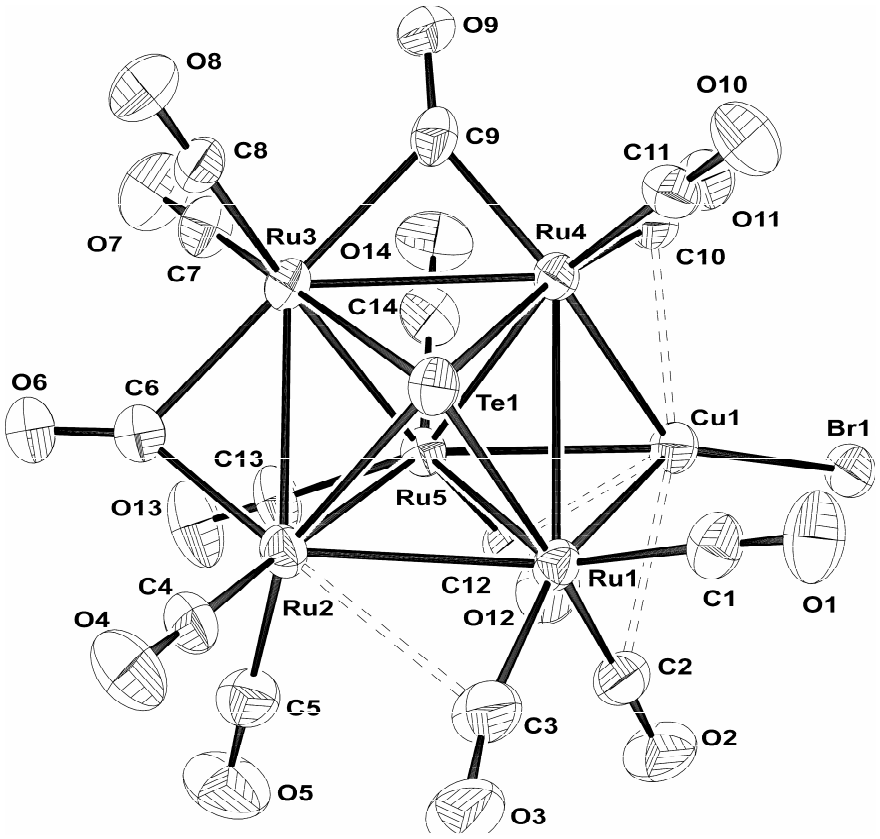


**Figure S2.** ORTEP diagram (30% thermal ellipsoids) showing the structure and atom labeling for the anion **2b**.

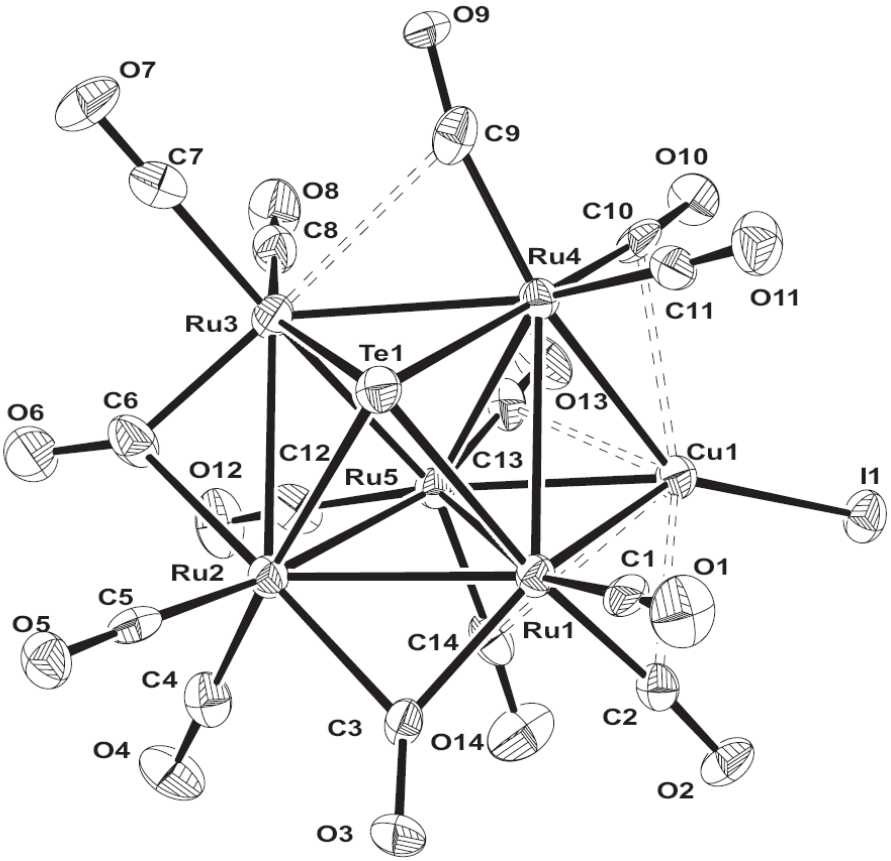


**Figure S3.** ORTEP diagram (30% thermal ellipsoids) showing the structure and atom labeling for the anion **2c**.

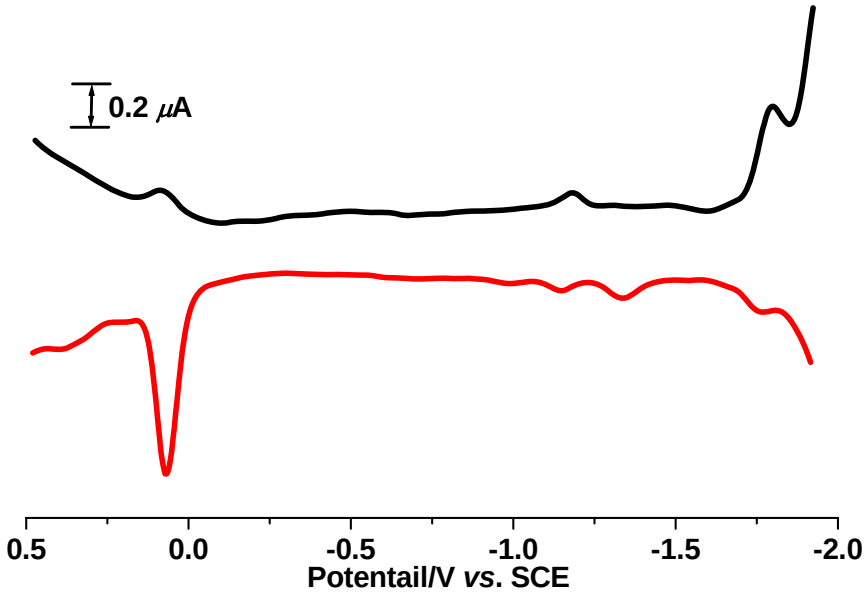


**Figure S4.** Differential pulse voltammetry in MeCN for $[PPh_4]_2$[**1**]. Conditions: electrolyte, 0.1 M $Bu_4NClO_4$; working electrode, glassy carbon; scan rate, 100 mV $s^{-1}$. Potentials are vs SCE.

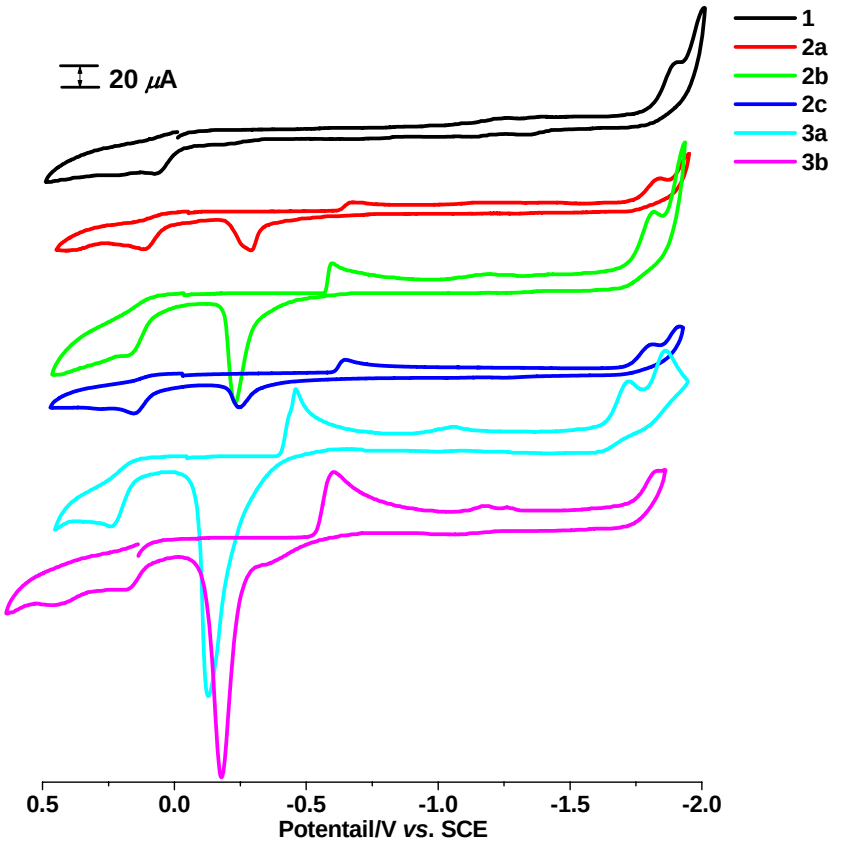


**Figure S5.** Cyclic voltammetry in MeCN for $[PPh_4]_2$[**1**], $[PPh_4]_2$[**2a**], $[PPh_4]_2$[**2b**], $[PPh_4]_2$[**2c**], $[PPh_4]_2$[**3a**], and $[PPh_4]_2$[**3b**]. Conditions: electrolyte, 0.1 M $Bu_4NClO_4$; working electrode, glassy carbon; scan rate, 100 mV $s^{-1}$. Potentials are vs SCE.

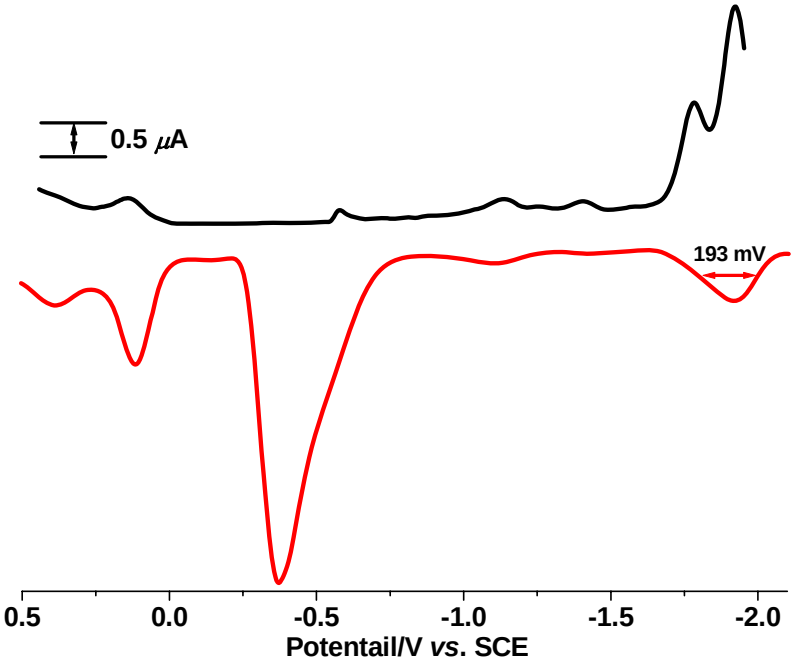


**Figure S6.** Differential pulse voltammetry in MeCN for $[PPh_4]_2$[**2b**]. Conditions: electrolyte, 0.1 M $Bu_4NClO_4$; working electrode, glassy carbon; scan rate, 100 mV $s^{-1}$. Potentials are vs SCE.

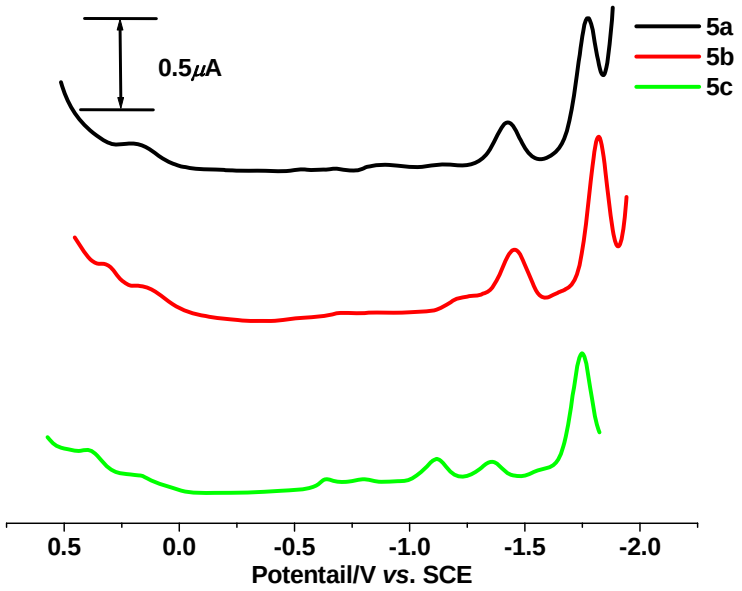


**Figure S7.** Differential pulse voltammetry in MeCN for $[PPh_4]_2$[**5a**], $[PPh_4]_2$[**5b**], and $[PPh_4]_2$[**5c**]. Conditions: electrolyte, 0.1 M $Bu_4NClO_4$; working electrode, glassy carbon; scan rate, 100 mV $s^{-1}$. Potentials are vs SCE.

**Computational Details:**

All calculations were performed using the LanL2DZ basis sets and applying the Becke-3-parameter density functional theory (DFT) and the Lee-Yang-Parr correlation functional (B3LYP).

$[TeRu_5(CO)_{14}]^{2-}$ (**1**)
E = –2064.3928976 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 8.70284 | 13.41216 | 6.95279 |
| Ru | 6.13072 | 14.02973 | 6.62844 |
| Ru | 7.33911 | 11.85469 | 5.18357 |
| Ru | 9.40986 | 13.54548 | 4.30037 |
| Ru | 8.27266 | 15.74777 | 5.69813 |
| Ru | 6.667 | 14.30516 | 3.85059 |
| O | 4.62255 | 16.60698 | 7.02587 |
| O | 5.19757 | 13.09417 | 9.34455 |
| O | 3.98255 | 12.48923 | 5.20014 |
| O | 7.69721 | 9.50197 | 7.02368 |
| O | 5.68663 | 10.06629 | 3.42895 |
| O | 9.57319 | 10.58412 | 3.66017 |
| O | 10.03402 | 13.5645 | 1.36547 |
| O | 12.35226 | 13.16438 | 4.8555 |
| O | 10.56406 | 16.52341 | 3.92628 |
| O | 6.78 | 18.15983 | 4.70718 |
| O | 9.5839 | 17.30762 | 7.92673 |
| O | 5.68043 | 12.53823 | 1.60541 |
| O | 7.93525 | 16.12498 | 1.83881 |
| O | 4.15069 | 15.99751 | 3.88266 |
| C | 5.22826 | 15.64667 | 6.85791 |
| C | 5.59129 | 13.43466 | 8.33681 |
| C | 4.96495 | 12.98327 | 5.53388 |
| C | 7.53987 | 10.41329 | 6.35622 |
| C | 6.30317 | 10.7755 | 4.0637 |
| C | 9.03113 | 11.51463 | 4.15095 |
| C | 9.77544 | 13.61373 | 2.47356 |

| | | | |
|---|---|---|---|
| C | 11.2446 | 13.31598 | 4.69191 |
| C | 9.76089 | 15.88748 | 4.4716 |
| C | 7.33508 | 17.22151 | 5.08672 |
| C | 9.08117 | 16.70163 | 7.10439 |
| C | 6.05764 | 13.1477 | 2.48447 |
| C | 7.52633 | 15.40817 | 2.62407 |
| C | 5.09487 | 15.34922 | 3.90229 |

$[TeRu_5(CO)_{14}CuCl]^{2-}$ (**2a**)
E = –2275.6222856 a.u.

| | x | y | z |
|---|---|---|---|
| Te | -0.12504 | 3.85161 | 4.70477 |
| Ru | 1.59587 | 4.84297 | 6.49732 |
| Ru | 0.52636 | 6.45934 | 4.42845 |
| Ru | -2.11325 | 5.71704 | 5.07285 |
| Ru | -1.241 | 3.98925 | 7.13498 |
| Ru | -0.45229 | 6.74823 | 7.15194 |
| Cu | 0.51607 | 4.82518 | 8.88761 |
| Cl | 1.16729 | 4.37786 | 10.93657 |
| O | 2.50179 | 2.00727 | 7.09153 |
| O | 3.44597 | 6.18604 | 8.50731 |
| O | 3.80097 | 5.30579 | 4.47163 |
| O | 2.28901 | 8.90096 | 4.72535 |
| O | 1.55539 | 6.04478 | 1.61764 |
| O | -1.63611 | 7.92977 | 2.94931 |
| O | -4.24116 | 7.79248 | 5.59584 |
| O | -3.78996 | 4.39993 | 2.91707 |
| O | -4.22438 | 4.13374 | 6.73127 |
| O | -2.24106 | 3.98718 | 9.99318 |
| O | -1.29479 | 0.95927 | 7.13078 |
| O | 0.98306 | 7.95846 | 9.55162 |
| O | -0.84849 | 9.53444 | 6.02478 |
| O | -3.07919 | 6.98904 | 8.67272 |
| C | 2.16154 | 3.07735 | 6.88266 |
| C | 2.66937 | 5.70133 | 7.80783 |
| C | 2.89973 | 5.18836 | 5.1627 |

| | | | |
|---|---|---|---|
| C | 1.60067 | 7.99598 | 4.63003 |
| C | 1.17311 | 6.18692 | 2.69139 |
| C | -1.20599 | 7.15855 | 3.71608 |
| C | -3.42063 | 6.9961 | 5.42483 |
| C | -3.1453 | 4.9076 | 3.71327 |
| C | -3.09376 | 4.37874 | 6.52942 |
| C | -1.76857 | 4.03309 | 8.94606 |
| C | -1.28219 | 2.10351 | 7.13498 |
| C | 0.52856 | 7.40621 | 8.63767 |
| C | -0.66322 | 8.45642 | 6.38364 |
| C | -2.0982 | 6.84203 | 8.08958 |

$[TeRu_5(CO)_{14}CuBr]^{2-}$ (**2b**)
E = –2273.8245727 a.u.

| | x | y | z |
|---|---|---|---|
| Te | -0.24521 | 3.91718 | 4.70512 |
| Ru | 1.50128 | 4.88389 | 6.48767 |
| Ru | 0.43755 | 6.51254 | 4.42559 |
| Ru | -2.21078 | 5.79956 | 5.0814 |
| Ru | -1.34514 | 4.05972 | 7.1432 |
| Ru | -0.52891 | 6.8154 | 7.1521 |
| Br | 1.12109 | 4.43211 | 11.04377 |
| Cu | 0.42727 | 4.89162 | 8.88578 |
| O | 2.41262 | 2.07963 | 7.13586 |
| O | 3.39634 | 6.24068 | 8.4311 |
| O | 3.7039 | 5.26941 | 4.43943 |
| O | 1.49374 | 6.06562 | 1.63283 |
| O | 2.20516 | 8.9379 | 4.71345 |
| O | -1.71439 | 7.9903 | 2.95209 |
| O | -4.30896 | 7.89116 | 5.6132 |
| O | -3.90668 | 4.54687 | 2.9309 |
| O | -4.32897 | 4.22044 | 6.76296 |
| O | -1.42444 | 1.0521 | 7.1401 |
| O | -2.33281 | 4.01725 | 10.0032 |
| O | 0.93262 | 8.02781 | 9.51589 |
| O | -0.93333 | 9.59211 | 6.06379 |

| | | | |
|---|---|---|---|
| O | -3.1148 | 7.05252 | 8.72773 |
| C | 2.05314 | 3.12592 | 6.90139 |
| C | 2.61645 | 5.76509 | 7.75876 |
| C | 2.78909 | 5.21136 | 5.13155 |
| C | 1.09159 | 6.23978 | 2.7049 |
| C | 1.51882 | 8.04255 | 4.63577 |
| C | -1.27301 | 7.23695 | 3.71483 |
| C | -3.49798 | 7.1003 | 5.44512 |
| C | -3.26336 | 5.00817 | 3.72754 |
| C | -3.20919 | 4.45622 | 6.56098 |
| C | -1.85814 | 4.07843 | 8.9509 |
| C | -1.40511 | 2.18234 | 7.1401 |
| C | 0.46758 | 7.4772 | 8.59495 |
| C | -0.74786 | 8.51635 | 6.40137 |
| C | -2.15782 | 6.92793 | 8.102 |

$[TeRu_5(CO)_{14}CuI]^{2-}$ (**2c**)

E = –2272.0389925 a.u.

| | x | y | z |
|---|---|---|---|
| I | 2.11271 | 9.28288 | 16.47594 |
| Te | 3.21259 | 2.66338 | 17.91083 |
| Ru | 4.28603 | 5.12821 | 17.71618 |
| Ru | 5.26703 | 3.02976 | 16.1257 |
| Ru | 2.64871 | 2.31572 | 15.29322 |
| Ru | 1.51127 | 4.4374 | 16.81868 |
| Ru | 3.59803 | 4.9839 | 14.89705 |
| Cu | 2.60306 | 6.8476 | 16.56651 |
| O | 4.29895 | 5.20603 | 20.75508 |
| O | 5.29733 | 7.97667 | 17.80632 |
| O | 7.26558 | 4.7198 | 17.77413 |
| O | 7.5538 | 3.60799 | 14.21587 |
| O | 6.9145 | 0.7306 | 17.20755 |
| O | 4.91867 | 0.8348 | 13.96692 |
| O | 1.44379 | -0.49174 | 15.43701 |
| O | 1.19869 | 2.84186 | 12.68569 |
| O | -0.60833 | 2.27661 | 16.48217 |

| | | | |
|---|---|---|---|
| O | -0.45774 | 6.34717 | 15.52071 |
| O | 0.54042 | 5.15166 | 19.58116 |
| O | 4.72231 | 3.75862 | 12.36806 |
| O | 1.55599 | 6.45511 | 13.16427 |
| O | 5.72246 | 7.13445 | 14.74811 |
| C | 4.27253 | 5.17371 | 19.63266 |
| C | 4.84918 | 6.93878 | 17.69258 |
| C | 6.17892 | 4.48186 | 17.42431 |
| C | 6.67463 | 3.41076 | 14.89189 |
| C | 6.26521 | 1.59126 | 16.82984 |
| C | 4.41014 | 1.60426 | 14.68801 |
| C | 1.89758 | 0.5524 | 15.40052 |
| C | 1.75345 | 2.6444 | 13.69651 |
| C | 0.27343 | 2.99155 | 16.5165 |
| C | 0.32096 | 5.6879 | 15.95637 |
| C | 0.92461 | 4.91019 | 18.53814 |
| C | 4.29852 | 4.1699 | 13.33811 |
| C | 2.29121 | 5.88929 | 13.90468 |
| C | 4.89432 | 6.32189 | 14.8597 |

$[\{TeRu_5(CO)_{14}\}_2Cu_4Cl_2]^{2-}$ (**3a**)

E = –4943.5672795 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 3.64991 | 7.73101 | 5.46703 |
| Ru | 6.10096 | 8.39975 | 6.35579 |
| Ru | 4.95187 | 9.73196 | 4.16011 |
| Ru | 4.35192 | 7.29652 | 2.85227 |
| Ru | 5.38616 | 5.75757 | 4.9674 |
| Ru | 6.98854 | 7.83444 | 3.64657 |
| Cu | 5.8949 | 6.04565 | 7.52378 |
| Cu | 7.8029 | 6.44442 | 5.79059 |
| Cl | 9.8865 | 5.6442 | 5.9526 |
| O | 8.80437 | 8.91411 | 7.61747 |
| O | 4.96006 | 8.9185 | 9.11376 |
| O | 6.22478 | 11.40759 | 6.41769 |
| O | 6.564 | 11.95922 | 2.94214 |

| | | | |
|---|---|---|---|
| O | 2.51688 | 11.50577 | 4.54389 |
| O | 4.14058 | 9.85397 | 1.21812 |
| O | 1.41062 | 6.81425 | 2.19935 |
| O | 5.44179 | 6.60805 | 0.11004 |
| O | 4.71386 | 4.24173 | 2.45917 |
| O | 7.31333 | 3.42478 | 4.91529 |
| O | 3.50423 | 3.7784 | 6.30153 |
| O | 9.59391 | 9.14421 | 4.51638 |
| O | 7.38658 | 9.27457 | 0.99804 |
| O | 8.15389 | 5.33355 | 2.37358 |
| C | 7.81565 | 8.64908 | 7.10088 |
| C | 5.36869 | 8.65409 | 8.08057 |
| C | 5.95859 | 10.36025 | 5.97751 |
| C | 5.98189 | 11.09793 | 3.38843 |
| C | 3.42297 | 10.83541 | 4.41703 |
| C | 4.30766 | 9.25807 | 2.21157 |
| C | 2.4807 | 6.98748 | 2.44083 |
| C | 5.02647 | 6.88274 | 1.13406 |
| C | 4.77673 | 5.18638 | 3.15 |
| C | 6.67038 | 4.37929 | 4.96725 |
| C | 4.19599 | 4.54812 | 5.84454 |
| C | 8.60399 | 8.64056 | 4.27184 |
| C | 7.17145 | 8.7607 | 1.98232 |
| C | 7.73113 | 6.24457 | 2.90546 |
| Cu | 6.9943 | 4.42313 | 9.49326 |
| Cl | 4.9107 | 5.22336 | 9.33125 |
| Ru | 8.69625 | 2.46781 | 8.92806 |
| Ru | 9.41104 | 5.10998 | 10.31644 |
| Ru | 7.80867 | 3.03311 | 11.63727 |
| Cu | 8.9023 | 4.8219 | 7.76007 |
| C | 6.98156 | 2.21847 | 8.18297 |
| C | 8.12682 | 6.48827 | 10.3166 |
| C | 6.19321 | 2.22699 | 11.01201 |
| Te | 11.14729 | 3.13655 | 9.81682 |
| Ru | 9.84533 | 1.13559 | 11.12374 |
| C | 9.42851 | 2.21347 | 7.20328 |
| C | 8.83862 | 0.5073 | 9.30634 |

| | | | |
|---|---|---|---|
| Ru | 10.44528 | 3.57103 | 12.43158 |
| C | 10.02047 | 5.68117 | 12.13385 |
| C | 10.60121 | 6.31943 | 9.4393 |
| C | 7.62576 | 2.10686 | 13.30153 |
| C | 7.06607 | 4.62299 | 12.37839 |
| O | 5.99283 | 1.95344 | 7.66638 |
| O | 7.48388 | 7.44278 | 10.36856 |
| O | 5.20329 | 1.72334 | 10.76747 |
| C | 8.81531 | -0.23037 | 11.89542 |
| C | 11.37423 | 0.03214 | 10.86682 |
| C | 10.48955 | 1.60949 | 13.07228 |
| O | 9.83715 | 1.94905 | 6.17009 |
| O | 8.57243 | -0.54004 | 8.86616 |
| C | 12.3165 | 3.88007 | 12.84302 |
| C | 9.77073 | 3.98482 | 14.14979 |
| O | 10.08335 | 6.62582 | 12.82468 |
| O | 11.29298 | 7.08916 | 8.98232 |
| O | 7.41063 | 1.59298 | 14.28581 |
| O | 6.64332 | 5.53401 | 12.91027 |
| O | 8.2332 | -1.09167 | 12.34171 |
| O | 12.28032 | -0.63822 | 10.73996 |
| O | 10.65663 | 1.01358 | 14.06573 |
| O | 13.38659 | 4.05331 | 13.0845 |
| O | 9.35541 | 4.25951 | 15.1738 |

$[\{TeRu_5(CO)_{14}\}_2Cu_4Br_2]^{2-}$ (**3b**)

E = –4940.0052068 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 1.37784 | 12.98229 | 2.18324 |
| Ru | -1.05295 | 12.30231 | 1.28834 |
| Ru | -0.36779 | 14.94197 | 2.70059 |
| Ru | 0.67818 | 13.39412 | 4.79338 |
| Ru | 0.09733 | 10.96983 | 3.47891 |
| Ru | -1.95139 | 12.8489 | 3.99871 |
| Cu | -0.85431 | 14.67045 | 0.14408 |
| Cu | -1.85705 | 16.3069 | -1.8584 |

| | | | |
|---|---|---|---|
| Br | 0.3173 | 15.48777 | -1.68728 |
| O | -3.73539 | 11.77319 | 0.00611 |
| O | 0.12013 | 11.79663 | -1.45305 |
| O | -1.15515 | 9.30191 | 1.20858 |
| O | -2.30853 | 17.2558 | 2.77317 |
| O | 1.50785 | 16.95671 | 1.42554 |
| O | 0.33107 | 16.44317 | 5.20714 |
| O | -0.38227 | 14.05273 | 7.51887 |
| O | 3.61865 | 13.89644 | 5.43479 |
| O | 0.94459 | 10.83397 | 6.39433 |
| O | -1.52008 | 8.72417 | 4.69987 |
| O | 2.55179 | 9.21842 | 3.09708 |
| O | -4.51749 | 11.50456 | 3.11542 |
| O | -3.18024 | 15.31547 | 5.2927 |
| O | -2.31319 | 11.40533 | 6.62657 |
| C | -2.77424 | 12.08002 | 0.54547 |
| C | -0.32837 | 12.05672 | -0.42476 |
| C | -0.9061 | 10.35248 | 1.68529 |
| C | -1.66476 | 16.28535 | 2.70594 |
| C | 0.8102 | 16.1743 | 1.85947 |
| C | 0.24407 | 15.52177 | 4.49513 |
| C | 0.03647 | 13.78371 | 6.48447 |
| C | 2.5406 | 13.71832 | 5.20561 |
| C | 0.74733 | 11.4448 | 5.43938 |
| C | -0.90198 | 9.59105 | 4.26441 |
| C | 1.63232 | 9.88777 | 3.20709 |
| C | -3.51288 | 12.0366 | 3.35683 |
| C | -2.72809 | 14.43883 | 4.75334 |
| C | -2.14454 | 11.95018 | 5.63037 |
| Cu | -2.76359 | 14.24567 | 1.8584 |
| Ru | -3.56769 | 18.25026 | -1.28834 |
| Ru | -4.25285 | 15.6106 | -2.70059 |
| Ru | -2.66925 | 17.70367 | -3.99871 |
| Cu | -3.76633 | 15.88212 | -0.14408 |
| Br | -4.93794 | 15.0648 | 1.68728 |
| Te | -5.99848 | 17.57028 | -2.18324 |
| Ru | -4.71797 | 19.58274 | -3.47891 |

| | | | |
|---|---|---|---|
| C | -1.8464 | 18.47255 | -0.54547 |
| C | -4.29227 | 18.49585 | 0.42476 |
| C | -3.71454 | 20.20009 | -1.68529 |
| Ru | -5.29882 | 17.15845 | -4.79338 |
| C | -2.95588 | 14.26722 | -2.70594 |
| C | -5.43085 | 14.37827 | -1.85947 |
| C | -4.86471 | 15.0308 | -4.49513 |
| C | -1.10777 | 18.51597 | -3.35683 |
| C | -1.89255 | 16.11374 | -4.75334 |
| C | -2.4761 | 18.60239 | -5.63037 |
| C | -5.36797 | 19.10777 | -5.43938 |
| C | -3.71866 | 20.96152 | -4.26441 |
| C | -6.25296 | 20.6648 | -3.20709 |
| O | -0.88525 | 18.77938 | -0.00611 |
| O | -4.74077 | 18.75594 | 1.45305 |
| O | -3.46549 | 21.25067 | -1.20858 |
| C | -4.65711 | 16.76886 | -6.48447 |
| C | -7.16124 | 16.83425 | -5.20561 |
| O | -2.31211 | 13.29677 | -2.77317 |
| O | -6.12849 | 13.59586 | -1.42554 |
| O | -4.95171 | 14.1094 | -5.20714 |
| O | -0.10315 | 19.04801 | -3.11542 |
| O | -1.4404 | 15.2371 | -5.2927 |
| O | -2.30745 | 19.14724 | -6.62657 |
| O | -5.56523 | 19.7186 | -6.39433 |
| O | -3.10056 | 21.8284 | -4.69987 |
| O | -7.17244 | 21.33415 | -3.09708 |
| O | -4.23837 | 16.49984 | -7.51887 |
| O | -8.23929 | 16.65613 | -5.43479 |

$[TeRu_5(CO)_{14}(CuCl)_2]^{2-}$ (**4a**) (the Optimized Geometry)
E = –2486.772994 a.u.

| | x | y | z |
|---|---|---|---|
| Te | -0.0137 | 1.120715 | -2.06804 |
| Ru | 0.017271 | -1.50706 | -1.24121 |
| Ru | 2.138675 | 0.669918 | -0.38402 |

| | | | |
|---|---|---|---|
| Ru | -0.02554 | 2.440911 | 0.466591 |
| Ru | -2.15313 | 0.625175 | -0.38205 |
| Ru | 0.003958 | -0.34738 | 1.510035 |
| Cu | -2.01129 | -1.97096 | 0.506654 |
| Cu | 2.052858 | -1.92769 | 0.510246 |
| O | -2.19216 | -2.20495 | -3.28544 |
| O | 0.039562 | -4.42009 | -0.17582 |
| O | 2.25405 | -2.16199 | -3.26974 |
| O | 4.019536 | 1.331522 | -2.71966 |
| O | 4.677771 | -0.08654 | 1.18149 |
| O | 2.949337 | 3.330063 | 0.808885 |
| O | -0.05353 | 5.237101 | -0.84315 |
| O | -0.03796 | 3.641507 | 3.288549 |
| O | -3.0181 | 3.270518 | 0.805753 |
| O | -4.67207 | -0.18087 | 1.19147 |
| O | -4.05124 | 1.239241 | -2.71674 |
| O | 0.029684 | -3.05167 | 3.030196 |
| O | 2.151735 | 0.717996 | 3.444936 |
| O | -2.16225 | 0.675944 | 3.447161 |
| C | -1.38434 | -1.9083 | -2.47629 |
| C | 0.029106 | -3.2715 | -0.44524 |
| C | 1.435821 | -1.88025 | -2.46566 |
| C | 3.28872 | 1.06419 | -1.82154 |
| C | 3.657073 | 0.087363 | 0.609164 |
| C | 2.147258 | 2.496248 | 0.454918 |
| C | -0.04279 | 4.160514 | -0.34959 |
| C | -0.03302 | 3.150855 | 2.212022 |
| C | -2.1993 | 2.452321 | 0.453625 |
| C | -3.65699 | 0.013387 | 0.615821 |
| C | -3.31344 | 0.990273 | -1.81904 |
| C | 0.020581 | -2.09809 | 2.329424 |
| C | 1.379171 | 0.342176 | 2.628602 |
| C | -1.38309 | 0.315931 | 2.629959 |
| Cl | 3.586629 | -3.55867 | 0.902494 |
| Cl | -3.51669 | -3.62945 | 0.894958 |

$[TeRu_5(CO)_{14}(CuBr)_2]^{2-}$ (**4b**)

E = –2483.1942675 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 3.40151 | 5.44743 | 16.32491 |
| Ru | 1.80538 | 3.3021 | 16.27869 |
| Ru | 2.04879 | 5.20962 | 13.99653 |
| Ru | 4.84323 | 4.94596 | 14.04451 |
| Ru | 4.81738 | 3.16254 | 16.2072 |
| Ru | 3.22846 | 2.56542 | 13.85141 |
| Br | 3.29957 | -1.14757 | 16.78044 |
| Br | -1.50976 | 2.36625 | 13.33438 |
| Cu | 3.24636 | 1.05778 | 16.13474 |
| Cu | 0.59796 | 2.98756 | 13.91682 |
| O | 1.94988 | 3.3624 | 19.31994 |
| O | 0.18244 | 0.77078 | 16.29416 |
| O | -0.82304 | 4.84036 | 16.37054 |
| O | 0.69706 | 7.86883 | 14.42581 |
| O | 0.26175 | 4.9352 | 11.59588 |
| O | 3.57639 | 6.7184 | 11.86027 |
| O | 6.59396 | 7.39865 | 14.44344 |
| O | 6.31324 | 4.08597 | 11.60959 |
| O | 7.5404 | 3.92114 | 15.23661 |
| O | 6.38468 | 0.59453 | 16.39404 |
| O | 5.84053 | 3.71917 | 18.97134 |
| O | 1.70499 | -0.03044 | 13.38001 |
| O | 3.00999 | 3.31448 | 10.92414 |
| O | 5.77935 | 1.07351 | 13.22138 |
| C | 1.90734 | 3.29365 | 18.16642 |
| C | 0.84516 | 1.63917 | 16.2119 |
| C | 0.1783 | 4.29468 | 16.27262 |
| C | 1.20972 | 6.86754 | 14.29068 |
| C | 0.87284 | 4.9198 | 12.53005 |
| C | 3.48248 | 5.96717 | 12.78465 |
| C | 5.91757 | 6.45148 | 14.27306 |
| C | 5.74926 | 4.46005 | 12.52026 |
| C | 6.39538 | 3.90189 | 15.2699 |
| C | 5.69306 | 1.50325 | 16.30591 |

| | | | |
|---|---|---|---|
| C | 5.42651 | 3.49865 | 17.96078 |
| C | 2.11854 | 0.95263 | 13.62873 |
| C | 3.02814 | 3.08471 | 12.00911 |
| C | 4.82907 | 1.62809 | 13.52298 |

$[TeRu_5(CO)_{14}(CuBr)_2]^{2-}$ (**4b**) (the Optimized Geometry)
E = –2483.209825 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 0.00061 | -1.49904 | 2.00842 |
| Ru | -0.00055 | 1.180766 | 1.380596 |
| Ru | 2.147418 | -0.90725 | 0.358698 |
| Ru | 0.001033 | -2.63743 | -0.60794 |
| Ru | -2.14669 | -0.90888 | 0.3587 |
| Ru | -0.00012 | 0.232134 | -1.44318 |
| Br | -3.67673 | 3.527351 | -0.55903 |
| Br | 3.674288 | 3.529911 | -0.55897 |
| Cu | -2.05592 | 1.751467 | -0.31349 |
| Cu | 2.054522 | 1.753082 | -0.31331 |
| O | -2.22003 | 1.695421 | 3.468071 |
| O | -0.00116 | 4.164808 | 0.535825 |
| O | 2.217838 | 1.696869 | 3.468882 |
| O | 4.036996 | -1.68797 | 2.650507 |
| O | 4.674434 | -0.05318 | -1.17421 |
| O | 2.982896 | -3.48185 | -0.99605 |
| O | 0.002027 | -5.51909 | 0.50036 |
| O | 0.001432 | -3.62649 | -3.51155 |
| O | -2.9802 | -3.48399 | -0.9963 |
| O | -4.6745 | -0.05662 | -1.17391 |
| O | -4.03557 | -1.69137 | 2.650485 |
| O | -0.00116 | 3.038193 | -2.7633 |
| O | 2.14888 | -0.67338 | -3.45612 |
| O | -2.14847 | -0.675 | -3.45607 |
| C | -1.40918 | 1.472492 | 2.638906 |
| C | -0.00083 | 2.999852 | 0.720161 |
| C | 1.4074 | 1.473437 | 2.639455 |
| C | 3.303188 | -1.37425 | 1.770382 |

| | | | |
|---|---|---|---|
| C | 3.659443 | -0.26187 | -0.6037 |
| C | 2.173099 | -2.67858 | -0.59269 |
| C | 0.001649 | -4.41082 | 0.08327 |
| C | 0.001275 | -3.21705 | -2.40174 |
| C | -2.17102 | -2.68017 | -0.59282 |
| C | -3.65927 | -0.26459 | -0.60354 |
| C | -3.30204 | -1.37697 | 1.770369 |
| C | -0.00078 | 2.035424 | -2.1351 |
| C | 1.378526 | -0.36362 | -2.61037 |
| C | -1.37836 | -0.36461 | -2.61033 |

$[TeRu_5(CO)_{14}(CuI)_2]^{2-}$ (**4c**) (the Optimized Geometry)
E = –2479.646844 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 0.001019 | -1.79812 | 1.97229 |
| Ru | -0.00035 | 0.904656 | 1.44503 |
| Ru | 2.146338 | -1.14222 | 0.343743 |
| Ru | 0.000937 | -2.83824 | -0.68132 |
| Ru | -2.14534 | -1.14376 | 0.344365 |
| Ru | -0.00017 | 0.068111 | -1.40669 |
| Cu | -2.07713 | 1.54383 | -0.21533 |
| Cu | 2.075894 | 1.545264 | -0.21542 |
| O | -2.21634 | 1.33198 | 3.556197 |
| O | -0.00128 | 3.919481 | 0.723312 |
| O | 2.214913 | 1.333577 | 3.556658 |
| O | 4.036853 | -1.98839 | 2.61179 |
| O | 4.672341 | -0.27088 | -1.17883 |
| O | 2.981315 | -3.67529 | -1.08873 |
| O | 0.002098 | -5.762 | 0.310503 |
| O | 0.000805 | -3.70435 | -3.6244 |
| O | -2.97892 | -3.6774 | -1.08793 |
| O | -4.67243 | -0.27416 | -1.17739 |
| O | -4.03468 | -1.99151 | 2.612795 |
| O | -0.00089 | 2.921383 | -2.61906 |
| O | 2.144557 | -0.76032 | -3.45678 |
| O | -2.1451 | -0.76151 | -3.4561 |

| | | | |
|---|---|---|---|
| C | -1.40781 | 1.14501 | 2.716161 |
| C | -0.0009 | 2.747984 | 0.859896 |
| C | 1.406635 | 1.146081 | 2.716502 |
| C | 3.302965 | -1.64927 | 1.741522 |
| C | 3.659413 | -0.48297 | -0.60601 |
| C | 2.170938 | -2.88462 | -0.66256 |
| C | 0.001662 | -4.63807 | -0.06177 |
| C | 0.000853 | -3.34242 | -2.49832 |
| C | -2.16897 | -2.88618 | -0.66197 |
| C | -3.65916 | -0.48551 | -0.60492 |
| C | -3.30124 | -1.65177 | 1.742384 |
| C | -0.00063 | 1.895403 | -2.0298 |
| C | 1.377118 | -0.48229 | -2.59747 |
| C | -1.37756 | -0.48299 | -2.59703 |
| I | -3.80924 | 3.449364 | -0.39884 |
| I | 3.806881 | 3.451904 | -0.39832 |

$[Te_2Ru_4(CO)_{10}(CuCl)_2]^{2-}$ (**5a**)
E = –1947.7571854 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 1.28574 | 1.55262 | 12.69561 |
| Ru | 2.03095 | 2.45881 | 15.18397 |
| Ru | 2.08479 | 4.165 | 12.97415 |
| Cu | 0.79154 | 4.87643 | 10.82354 |
| Cl | 1.0431 | 5.96816 | 8.99501 |
| O | 3.85494 | 0.07531 | 15.52185 |
| O | 2.63928 | 3.46412 | 17.95842 |
| O | 4.57885 | 4.07076 | 14.71561 |
| O | 2.42759 | 7.16532 | 13.02072 |
| O | 4.1996 | 3.98551 | 10.8245 |
| C | 3.16156 | 0.98118 | 15.3996 |
| C | 2.36127 | 3.05969 | 16.92693 |
| C | 3.48926 | 3.74361 | 14.42855 |
| C | 2.28039 | 6.02637 | 13.00149 |
| C | 3.37913 | 4.03109 | 11.60876 |
| Ru | -0.74217 | 3.35542 | 12.2859 |

| | | | |
|---|---|---|---|
| Ru | -0.796 | 1.64923 | 14.49571 |
| Te | 0.00304 | 4.26161 | 14.77425 |
| C | -1.87278 | 4.83305 | 12.07026 |
| C | -1.07248 | 2.75454 | 10.54293 |
| C | -2.20048 | 2.07062 | 13.04132 |
| Cu | 0.49724 | 0.9378 | 16.64632 |
| C | -0.99161 | -0.21214 | 14.46838 |
| C | -2.09035 | 1.78314 | 15.8611 |
| O | -2.56616 | 5.73892 | 11.94802 |
| O | -1.35049 | 2.35011 | 9.51144 |
| O | -3.29007 | 1.74347 | 12.75426 |
| Cl | 0.24568 | -0.15393 | 18.47486 |
| O | -1.1388 | -1.35109 | 14.44915 |
| O | -2.91081 | 1.82872 | 16.64536 |

$[Te_2Ru_4(CO)_{10}(CuBr)_2]^{2-}$ (**5b**)
E = –1944.1996339 a.u.

| | x | y | z |
|---|---|---|---|
| Te | 3.8464 | 1.33255 | 1.05239 |
| Ru | 5.88487 | -0.45722 | 1.45304 |
| Ru | 5.93846 | 1.27806 | -0.73512 |
| Br | 4.92474 | 3.23619 | -4.75823 |
| Cu | 4.6455 | 2.01487 | -2.86903 |
| O | 6.46692 | 0.46533 | 4.26172 |
| O | 7.71271 | -2.85213 | 1.77017 |
| O | 8.41698 | 1.18078 | 1.01688 |
| O | 8.06514 | 1.13909 | -2.86612 |
| O | 6.26237 | 4.27346 | -0.65896 |
| C | 6.20196 | 0.06073 | 3.19768 |
| C | 7.03666 | -1.93137 | 1.66196 |
| C | 7.33604 | 0.84343 | 0.75052 |
| C | 7.21735 | 1.18237 | -2.09618 |
| C | 6.11128 | 3.1374 | -0.71722 |
| Ru | 3.11613 | 0.45722 | -1.45304 |
| Ru | 3.06254 | -1.27806 | 0.73512 |
| Te | 5.1546 | -1.33255 | -1.05239 |

| | | | |
|---|---|---|---|
| C | 2.79904 | -0.06073 | -3.19768 |
| C | 1.96434 | 1.93137 | -1.66196 |
| C | 1.66496 | -0.84343 | -0.75052 |
| Cu | 4.3555 | -2.01487 | 2.86903 |
| C | 1.78365 | -1.18237 | 2.09618 |
| C | 2.88972 | -3.1374 | 0.71722 |
| O | 2.53408 | -0.46533 | -4.26172 |
| O | 1.28829 | 2.85213 | -1.77017 |
| O | 0.58402 | -1.18078 | -1.01688 |
| Br | 4.07627 | -3.23619 | 4.7582 |
| O | 0.93586 | -1.13909 | 2.86612 |
| O | 2.73863 | -4.27346 | 0.65896 |

$[Te_2Ru_4(CO)_{10}(CuI)_2]^{2-}$ (**5c**)
E = –1940.6309079 a.u.

| | x | y | z |
|---|---|---|---|
| I | -2.50966 | 8.07702 | 4.45089 |
| Te | -1.08221 | 13.13468 | 1.22532 |
| Ru | -3.30347 | 11.53591 | 1.27181 |
| Ru | -0.52821 | 10.49369 | 0.73829 |
| Cu | -2.12353 | 9.61531 | 2.59564 |
| O | 2.07787 | 10.47471 | -0.80556 |
| O | -3.9434 | 11.98415 | 4.18401 |
| O | -5.58348 | 9.58398 | 1.23479 |
| O | -0.44658 | 7.48207 | 0.39602 |
| O | 1.31465 | 10.34817 | 3.12879 |
| C | 1.00703 | 10.87825 | -0.58911 |
| C | -3.66539 | 11.79587 | 3.09066 |
| C | -4.6977 | 10.29572 | 1.24217 |
| C | -0.49499 | 8.62069 | 0.53991 |
| C | 0.60222 | 10.38754 | 2.23836 |
| Ru | -0.18953 | 12.41653 | -1.27181 |
| Ru | -2.96479 | 13.45876 | -0.73829 |
| Te | -2.41079 | 10.81777 | -1.22532 |
| Cu | -1.36947 | 14.33714 | -2.59564 |
| C | 0.17239 | 12.15657 | -3.09066 |

| | | | |
|---|---|---|---|
| C | 1.2047 | 13.65673 | -1.24217 |
| C | -4.50003 | 13.07419 | 0.58911 |
| C | -2.99801 | 15.33176 | -0.53991 |
| C | -4.09522 | 13.56491 | -2.23836 |
| I | -0.98334 | 15.87543 | -4.45089 |
| O | 0.4504 | 11.9683 | -4.18401 |
| O | 2.09048 | 14.36847 | -1.23479 |
| O | -5.57087 | 13.47774 | 0.80556 |
| O | -3.04643 | 16.47038 | -0.39602 |
| O | -4.80765 | 13.60428 | -3.12879 |