Supporting Information

En Route to Osmium Analogs of KP1019: Synthesis, Structure, Spectroscopic Properties and Antiproliferative Activity of trans-[Os^{IV}Cl_{4}(Hazole)_{2}]

Gabriel E. Büchel, Iryna N. Stepanenko, Michaela Hejl, Michael A. Jakupec, Bernhard K. Keppler, Vladimir B. Arion*

University of Vienna, Institute of Inorganic Chemistry, Währinger Strasse 42, A-1090
Vienna, Austria

RECEIVED DATE (to be automatically inserted after your manuscript is accepted)

To whom correspondence should be addressed. E-mail: vladimir.arion@univie.ac.at (V.B.A.)
Figure S1: Thermogravimetric data for (H$_2$ind)$_2$[OsCl$_6$] and (H$_2$ind)[OsCl$_5$(κN$_2$-Hind)] showing a weight loss of 11.29% and 6.22%, respectively, attributed to the loss of one (calcd. weight loss 6.03%) and two (calcd. weight loss 11.37%) molecules of HCl.
Figure S2. The unit cell of 1 showing the formation of a chain along axis $a$ via intermolecular hydrogen bonding interaction N2–H···Cl2$^i$ [N2–H 0.88, H···Cl2$^i$ 2.511, N2···Cl2$^i$ 3.270 Å, N2–H···Cl2$^i$ 144.9°] (symmetry code $i$: $x$–1, $y$, $z$).

Figure S3. The unit cell of 2; hydrogen atoms were omitted for clarity.
Figure S4. Bifurcated hydrogen bonding interactions N2–H···Cl1\textsuperscript{i} and N2–H···Cl2\textsuperscript{ii} [N2–H 0.88, H···Cl1\textsuperscript{i} 2.798, N2···Cl1\textsuperscript{i} 3.444 Å, N2–H···Cl1\textsuperscript{i} 131.5°; H···Cl2\textsuperscript{ii} 2.713, N2···Cl2\textsuperscript{ii} 3.143 Å, N2–H···Cl2\textsuperscript{ii} 111.4°] (symmetry codes i: x, –y + 1.5, z – 0.5; ii: –x, –y + 2, –z) and π–π stacking interaction in the crystal structure of 2.

Figure S5. Strong hydrogen bonding N4–H···O1\textsuperscript{i} [N4–H 0.88, H···O1\textsuperscript{i} 1.826, N4···O1\textsuperscript{i} 2.698 Å, N4–H···O1\textsuperscript{i} 170.9°] (symmetry code i: x + 1, y, z) between molecule of 3 and DMSO.
Figure S6. Bifurcated hydrogen bonding interactions N2–H···Cl1\textsuperscript{i} and N2–H···Cl2\textsuperscript{ii} [N2–H 0.88, H···Cl1\textsuperscript{i} 2.867, N2···Cl1\textsuperscript{i} 3.541 Å, N2–H···Cl1\textsuperscript{i} 134.6°; H···Cl2\textsuperscript{ii} 2.770, N2···Cl2\textsuperscript{ii} 3.504 Å, N2–H···Cl2\textsuperscript{ii} 141.9°] (symmetry codes i: –x + 1, y + 0.5, –z + 0.5; ii: x, –y + 0.5, z – 0.5) and π–π stacking interaction in the crystal structure of 4.

Figure S7: UV–vis spectra of 1 (red), 2 (blue), 3 (green) and 4 (black) in DMSO.