Titanium oxo-clusters derivatized from the $Ti_{10}O_{12}(cat)_8(py)_8$ complex: Structural investigation and spectroscopic studies of light absorption

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Supporting information

Table 1: Ti-N bond lengths measured from the structures of $Ti_{10}O_{12}(cat)_8(py)_8$, $Ti_{10}O_{12}(cat)_8(pico)_8$, $Ti_{10}O_{12}(cat)_8(4\text{-}Phpy)_8$ and $Ti_{10}O_{12}(cat)_8(pyrald)_8$.

	Ti-N bond	Distance (Å)
$Ti_{10}O_{12}(cat)_8(py)_8$	Ti1-N2	2.226(2)
	Ti2-N1	2.228(8)
$Ti_{10}O_{12}(cat)_8(pico)_8$	Ti1-N1	2.294(5)
	Ti2-N2	2.239(5)
	Ti3-N3	2.281(5)
	Ti4-N4	2.249(5)
	Ti5-N5	2.269(4)
	Ti7-N6	2.256(5)
	Ti9-N7	2.249(4)
	Ti10-N8	2.271(6)
$Ti_{10}O_{12}(cat)_8(4\text{-}Phpy)_8$	Ti1-N1	2.293(4)
	Ti3-N2	2.272(4)
$Ti_{10}O_{12}(cat)_8(pyrald)_8$	Ti1-N1	2.25(1)
	Ti2-N2	2.31(1)

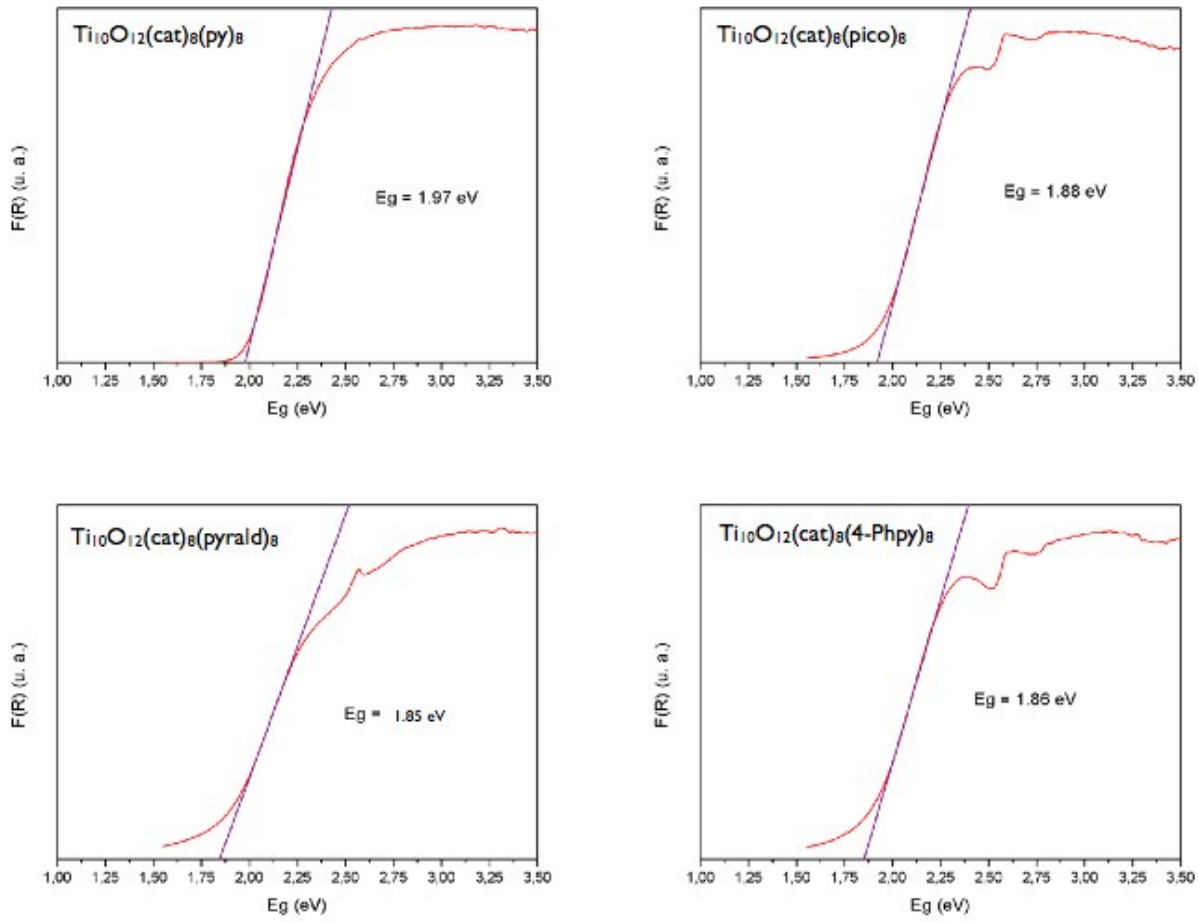

Figure 1 : Band gaps in $Ti_{10}O_{12}(cat)_8(py)_8$, $Ti_{10}O_{12}(cat)_8(pico)_8$, $Ti_{10}O_{12}(cat)_8(pyrald)_8$, and $Ti_{10}O_{12}(cat)_8(4\text{-}Phpy)_8$ determined by using direct analysis of the absorption edges.

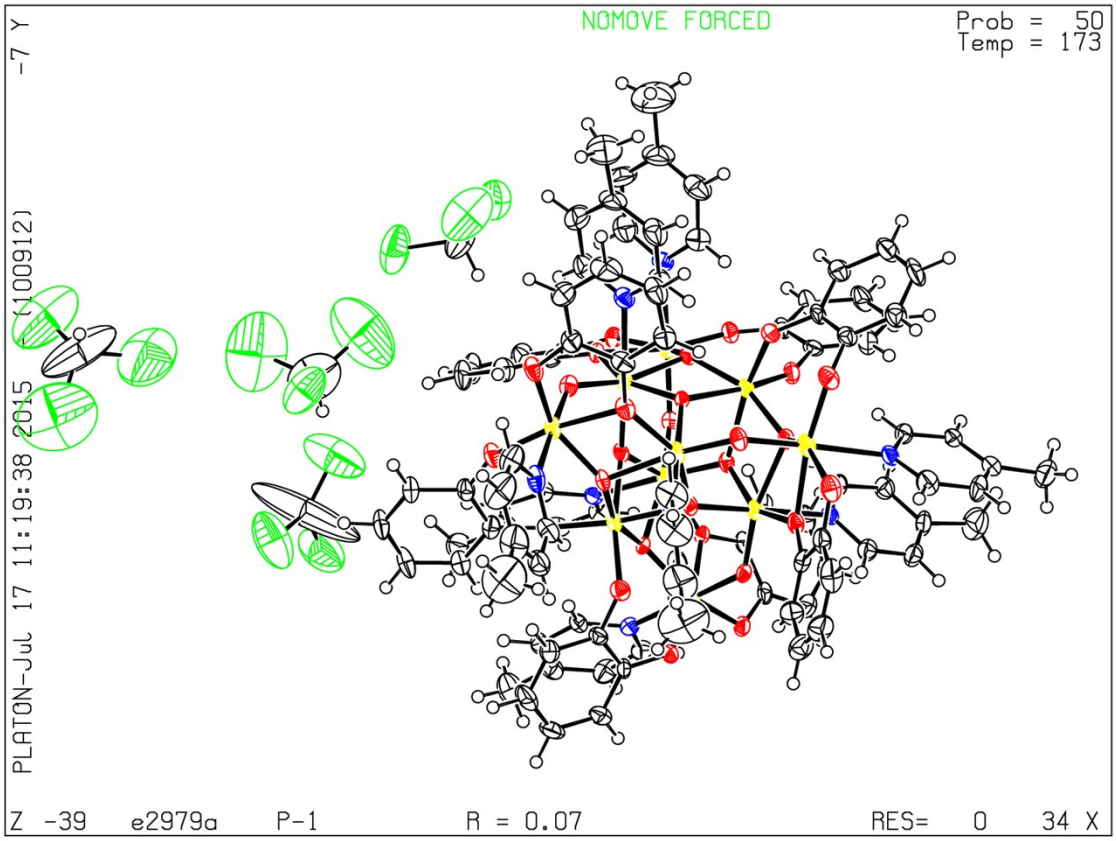

Figure 2 : Ellipsoid plot of the $Ti_{10}O_{12}(cat)_8(pico)_8$ structure

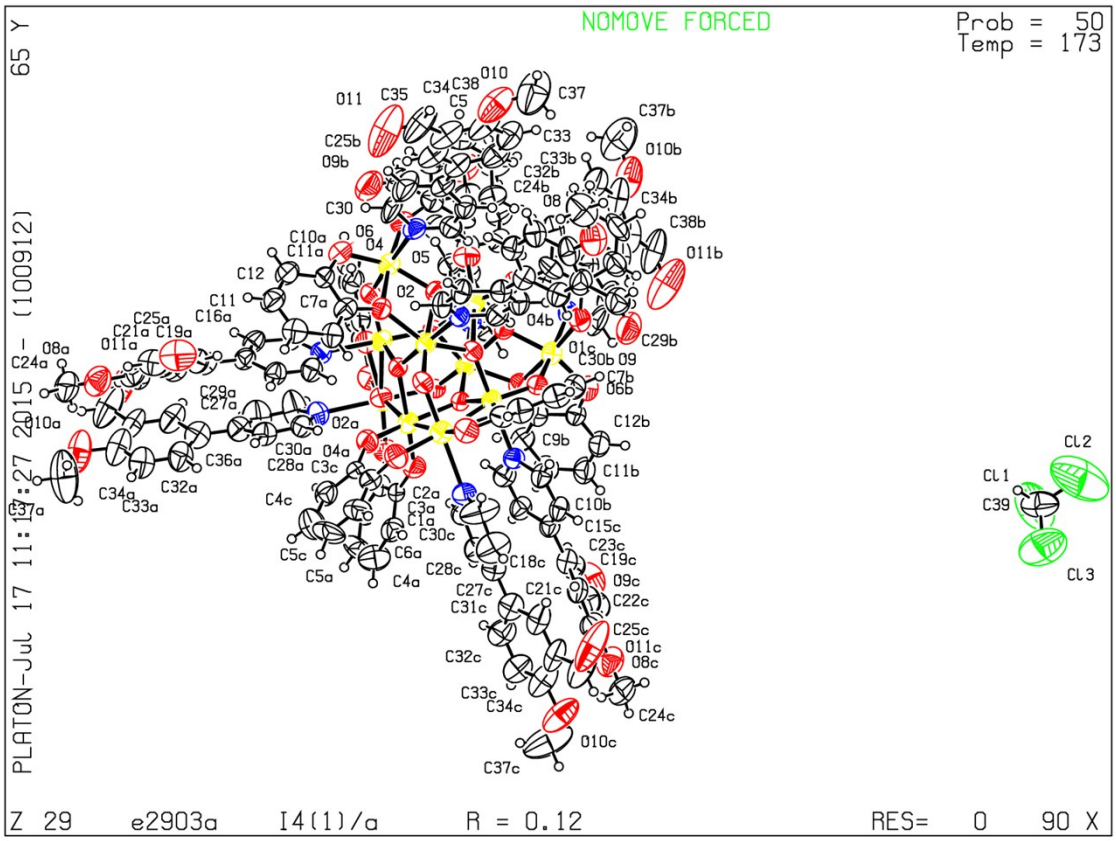

Figure 3: Ellipsoid plot of the $Ti_{10}O_{12}(cat)_8(pyrald)_8$ structure

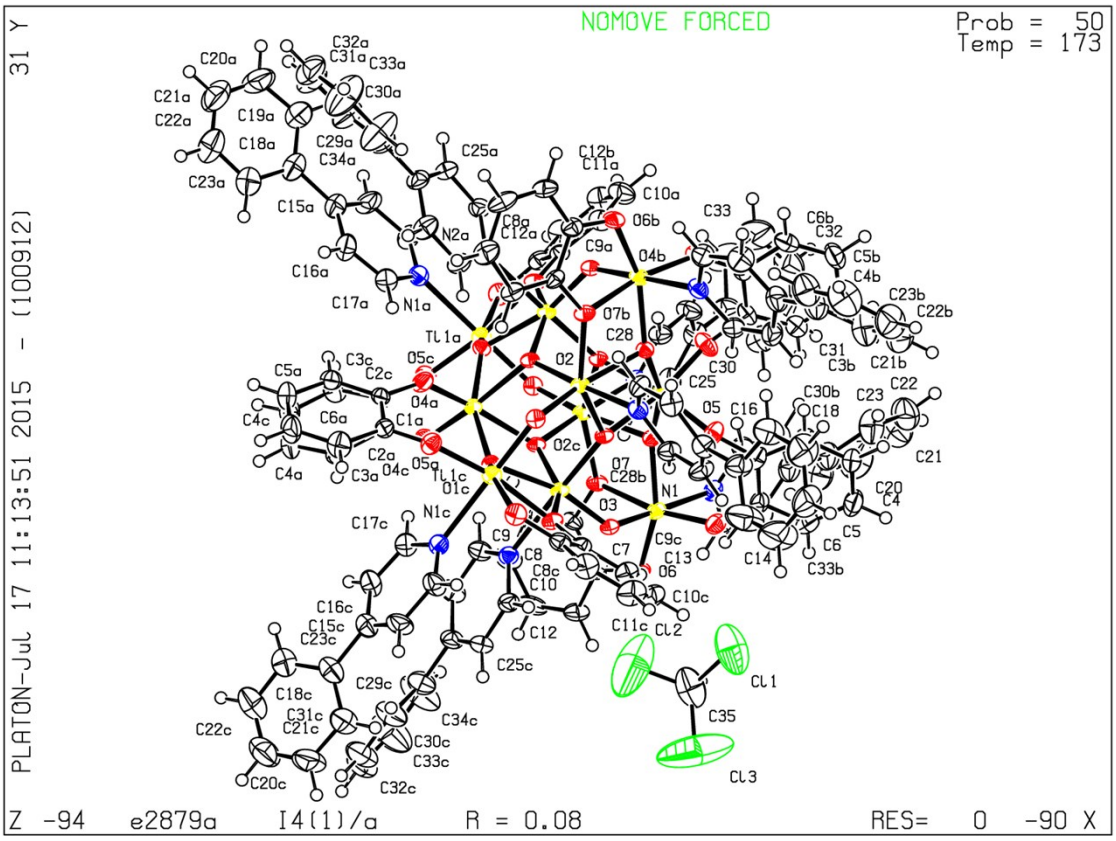

Figure 4: Ellipsoid plot of the $Ti_{10}O_{12}(cat)_8(4\text{-Phpy})_8$ structure