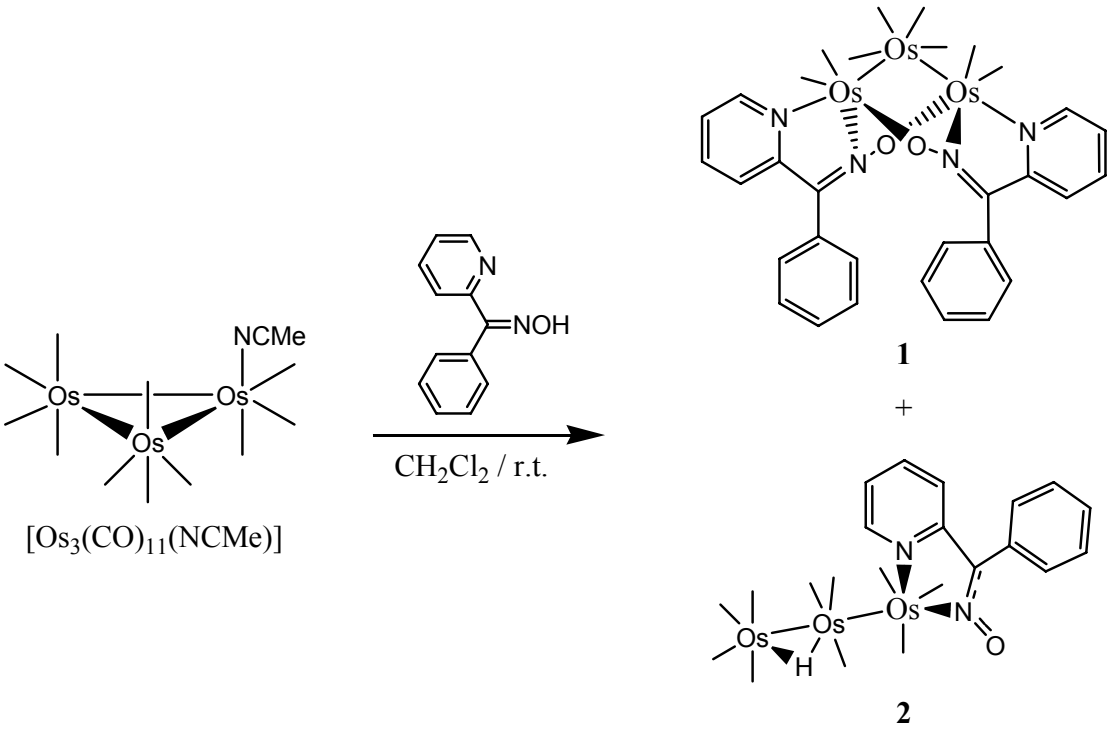
Electronic Supplementary Material for CrystEngComm

Electronic Supplementary information

An Open-Channel Architecture Assembly from the $[Os_3(CO)_8\{\mu\text{-}\eta^3\text{-}ON{=}CPh(NC_5H_4)\}_2]$ Cluster

Janet Shuk-Yee Wong, Yan-Juan Gu, Lap Szeto and Wing-Tak Wong*

Synthesis of the compound $[Os_3(CO)_8\{\mu\text{-}\eta^3\text{-}ON{=}CPh(NC_5H_4)\}_2]$ cluster



Scheme S1 Reaction of $[Os_3(CO)_{11}(NCMe)]$ with phenyl 2-pyridyl ketoxime.

Table S1 Selected bond distances (Å) and angles (°) of crystals **a** and **b.**

Bond lengths	**a**	**b**
Os1-Os2	2.8232(7)	2.8443(8)
Os1-N1	2.147(6)	2.161(5)
Os1-N2	2.133(6)	2.131(5)
Os1*-O5	2.120(5)	2.108(4)
N2-O5	1.347(8)	1.348(6)
N1-C5	1.336(10)	1.345(7)
N1-C9	1.353(9)	1.374(7)
N2-C10	1.297(9)	1.300(7)
C9-C10	1.484(11)	1.462(8)
Bond angles		
Os1-Os2-Os1*	78.86(2)	78.66(3)
Os2-Os1-N2	93.90(17)	92.33(13)
Os2-Os1-O5*	90.40(14)	89.09(11)
Os1-N1-C5	127.2(5)	127.5(4)
Os1-N1-C9	116.0(5)	114.3(4)
Os1-N2-O5	124.7(5)	125.7(3)
Os1-N2-C10	118.1(5)	118.1(4)
Os1*-O5-N2	112.1(4)	111.9(3)
N1-Os1-N2	74.9(2)	74.56(18)
N1-C9-C10	114.3(7)	115.0(5)
N2-C10-C9	115.6(7)	115.3(5)
N2-C10-C11	122.5(7)	122.0(5)
O5-N2-C10	117.2(6)	116.1(5)

* Symmetry code for **a**: y, x, 1/2-z; and **b**: 1-y, 1-x, 1/2-z

Fig. S1 Unit cell of packing diagram in ball and stick form_(upper) and space-filling (lower) of crystal **b** viewed down the *c-axis*.

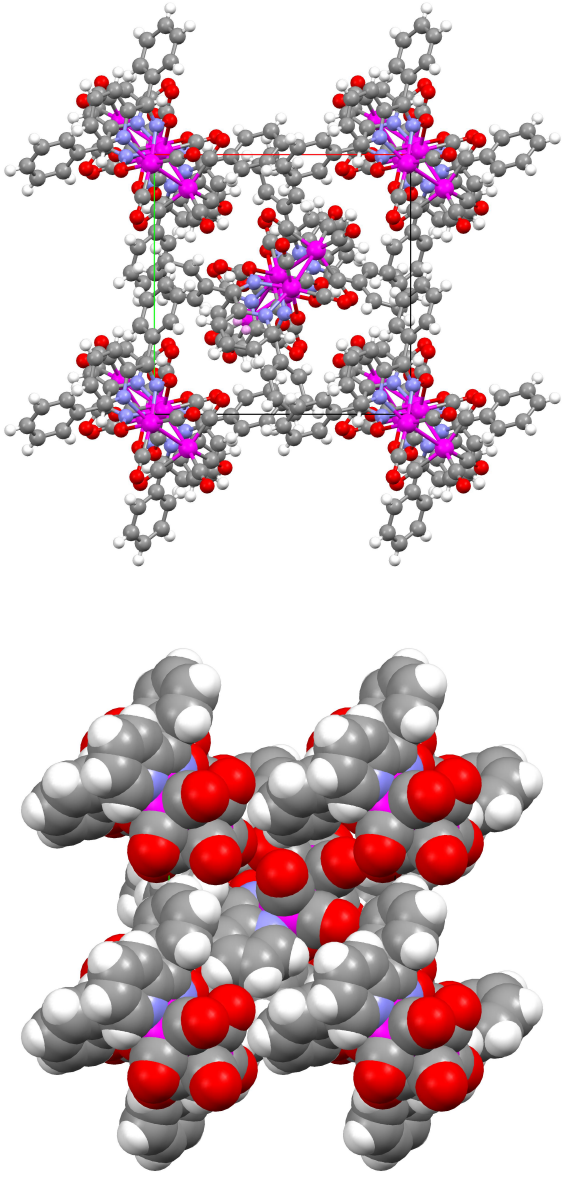


Fig. S2 IR spectrum of compound **a** in solution.

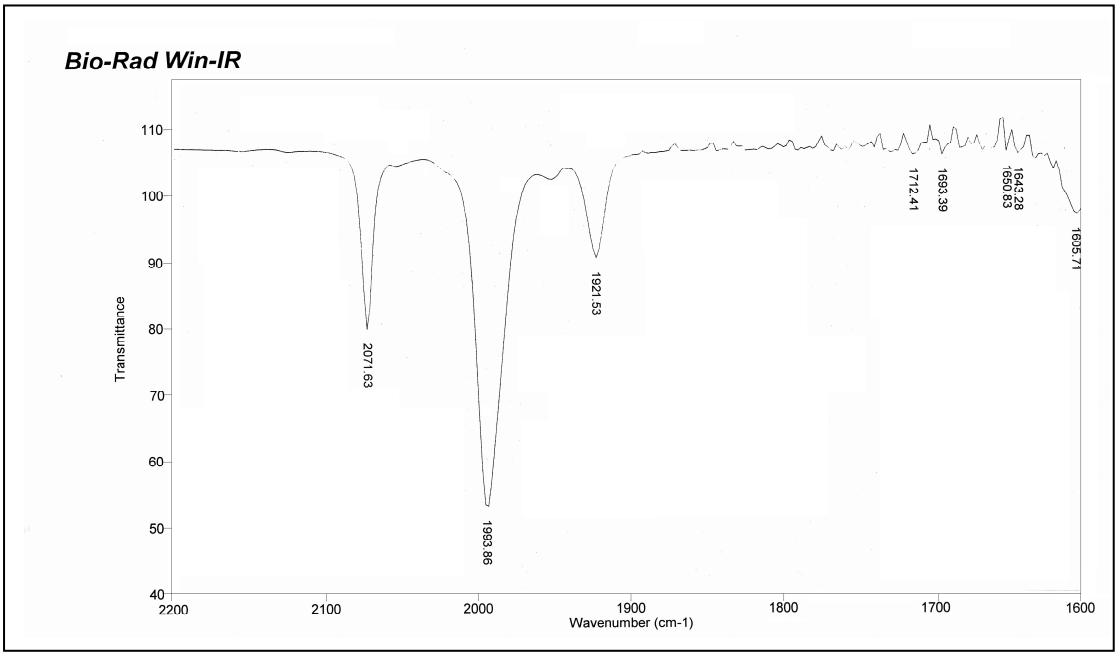


Fig. S3 Powder XRD of compound **a** using Copper Kα_1 radiation, 0-50°.

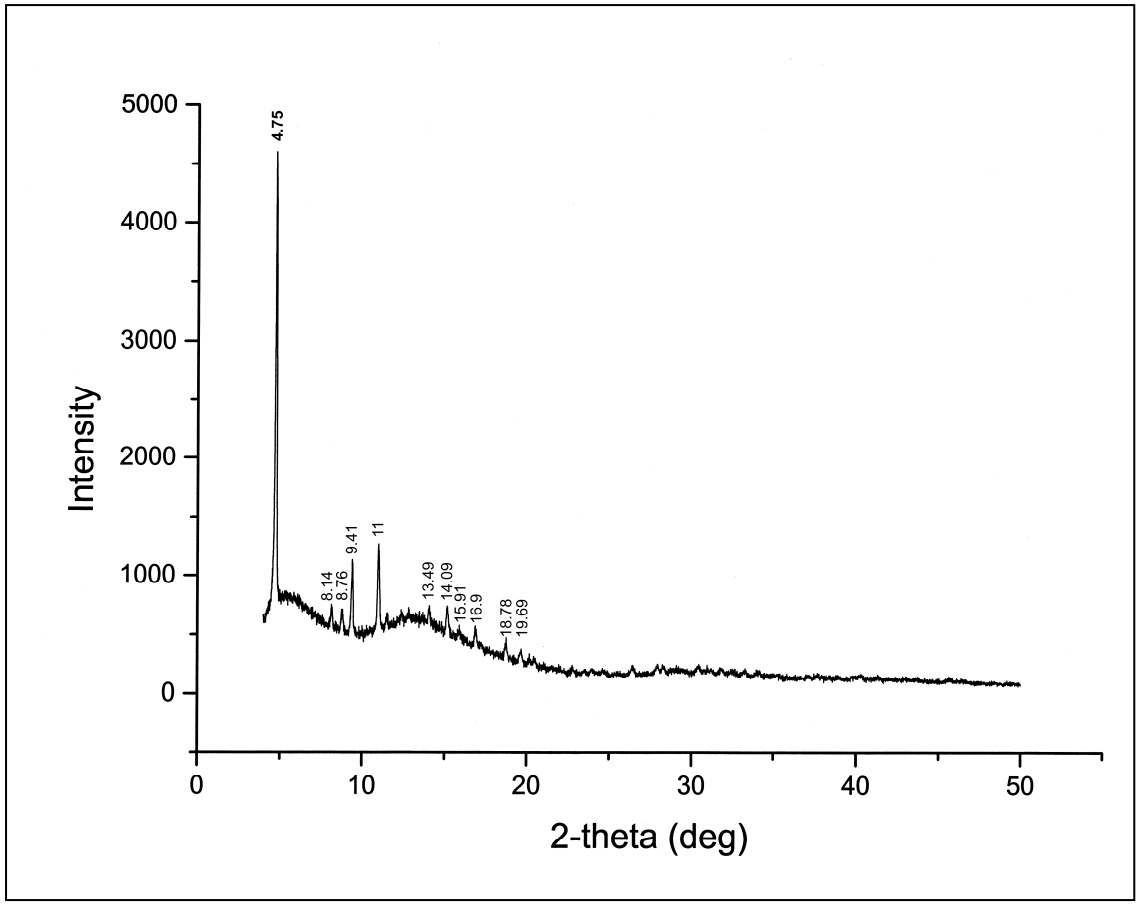


Fig. S4 Simulated Powder XRD of compound **a** using Copper Kα_1 radiation.

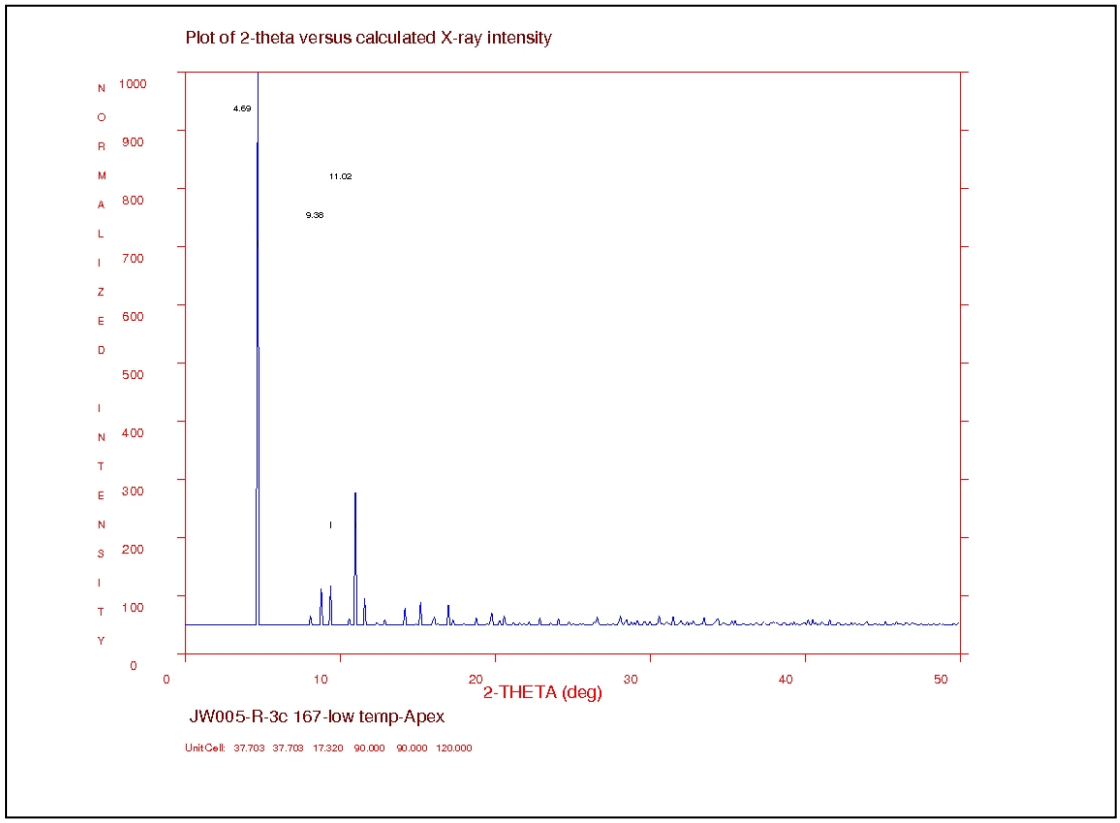


Fig. S5 Simulated Powder XRD of compound **b** using Copper Kα_1 radiation from 0-50°.