Electronic Supplementary Information

New Fe-Ta and Co-Ta oxalate complexes: structural characterization and thermal behaviour – formation of mixed-metal oxides

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Compound **1**: $[Fe(phen)_3][Ta(OC_2H_5)(C_2O_4)_3]\cdot H_2O$

Compound **2**: $[Co(phen)_3][Ta(OC_2H_5)(C_2O_4)_3]\cdot H_2O$

Compound **3**: $[Ni(phen)_3][Ta(OC_2H_5)(C_2O_4)_3]\cdot H_2O$ (L. Androš, D. Matković-Čalogović and P. Planinić, *CrystEngComm*, 2013, **15**, 533–543.)

Table S1 Selected bond lengths (Å) and angles (°) for the $[Fe(phen)_3]^{2+}$ cations in compound **1** and for the $[Co(phen)_3]^{2+}$ cations in compound **2**.

$[Fe(phen)_3]^{2+}$ cation		$[Co(phen)_3]^{2+}$ cation	
Fe1–N1	1.972(3)	Co1–N1	2.133(3)
Fe1–N2	1.987(2)	Co1–N2	2.110(3)
Fe1–N3	1.983(4)	Co1–N3	2.135(3)
Fe1–N4	1.974(3)	Co1–N4	2.154(3)
Fe1–N5	1.978(3)	Co1–N5	2.146(3)
Fe1–N6	1.986(3)	Co1–N6	2.124(3)
N1–Fe1–N2	82.44(12)	N1–Co1–N2	78.81(12)
N1–Fe1–N3	93.32(12)	N1–Co1–N3	98.47(12)
N1–Fe1–N4	173.79(12)	N1–Co1–N4	175.08(12)
N1–Fe1–N5	95.12(13)	N1–Co1–N5	92.59(12)
N1–Fe1–N6	90.02(12)	N1–Co1–N6	90.40(12)
N2–Fe1–N3	90.15(12)	N2–Co1–N3	92.52(11)
N2–Fe1–N4	92.78(12)	N2–Co1–N4	97.56(11)
N2–Fe1–N5	176.06(13)	N2–Co1–N5	169.52(12)
N2–Fe1–N6	94.25(12)	N2–Co1–N6	95.55(12)
N3–Fe1–N4	82.68(12)	N3–Co1–N4	78.26(12)
N3–Fe1–N5	93.09(12)	N3–Co1–N5	94.68(11)
N3–Fe1–N6	174.80(12)	N3–Co1–N6	169.03(12)
N4–Fe1–N5	89.86(12)	N4–Co1–N5	91.36(11)
N4–Fe1–N6	94.31(12)	N4–Co1–N6	93.28(12)
N5–Fe1–N6	82.63(13)	N5–Co1–N6	78.39(12)

Table S2 Selected bond lengths (Å) and angles (°) for the $[Ta(OC_2H_5)(C_2O_4)_3]^{2-}$ anion in compounds **1** and **2**.

	1	**2**
Ta1–O1	1.852(3)	1.861(3)
Ta1–O2	2.033(3)	2.031(3)
Ta1–O5	2.085(3)	2.086(2)
Ta1–O6	2.112(4)	2.128(3)
Ta1–O9	2.053(3)	2.044(3)
Ta1–O10	2.050(3)	2.057(3)
Ta1–O13	2.126(3)	2.114(3)
O1–Ta1–O2	161.74(12)	162.44(12)
O1–Ta1–O5	85.11(11)	85.72(11)
O1–Ta1–O6	93.31(14)	90.38(13)
O1–Ta1–O9	97.17(12)	98.66(13)
O1–Ta1–O10	100.50(14)	98.97(13)
O1–Ta1–O13	89.70(13)	92.80(14)
O2–Ta1–O5	76.79(10)	76.89(11)
O2–Ta1–O6	83.29(14)	82.03(13)
O2–Ta1–O9	98.89(12)	94.20(13)
O2–Ta1–O10	92.95(13)	96.53(13)
O2–Ta1–O13	82.45(13)	84.01(14)
O5–Ta1–O6	71.43(11)	71.83(11)
O5–Ta1–O9	144.05(12)	144.40(12)
O5–Ta1–O10	144.28(12)	143.88(11)
O5–Ta1–O13	71.82(11)	71.44(11)
O6–Ta1–O9	72.62(12)	72.82(12)
O6–Ta1–O10	142.15(12)	143.26(12)
O6–Ta1–O13	142.70(12)	142.73(12)
O9–Ta1–O10	70.80(12)	70.67(12)
O9–Ta1–O13	143.75(12)	142.77(12)
O10–Ta1–O13	72.96(12)	72.56(12)

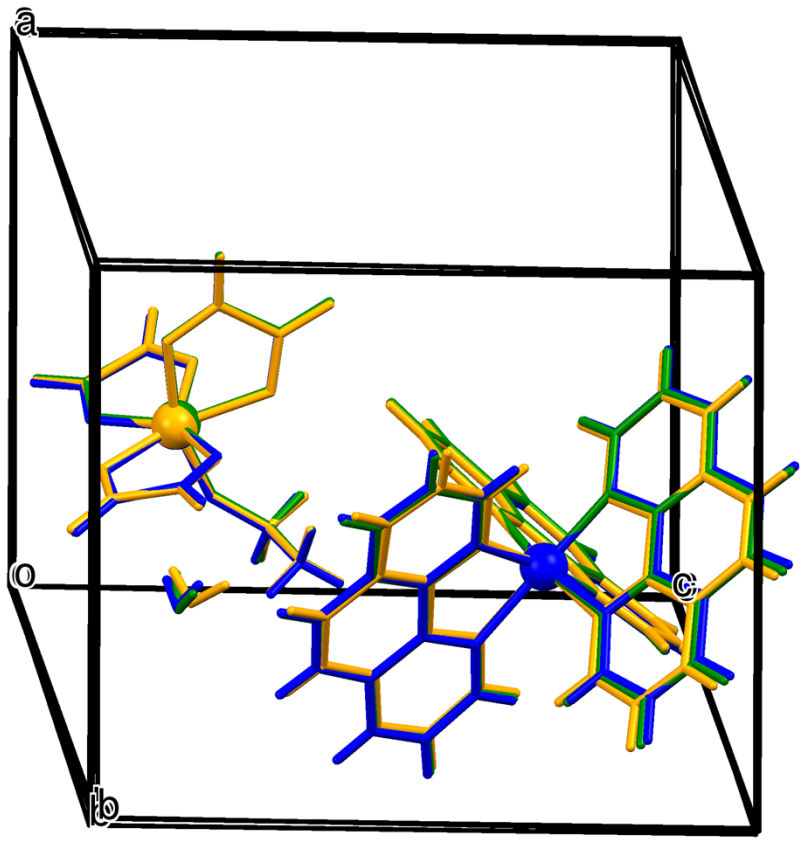

Fig. S1 Unit cells and asymmetric units overlay of isostructural compounds **1** (orange), **2** (blue) and **3** (green).

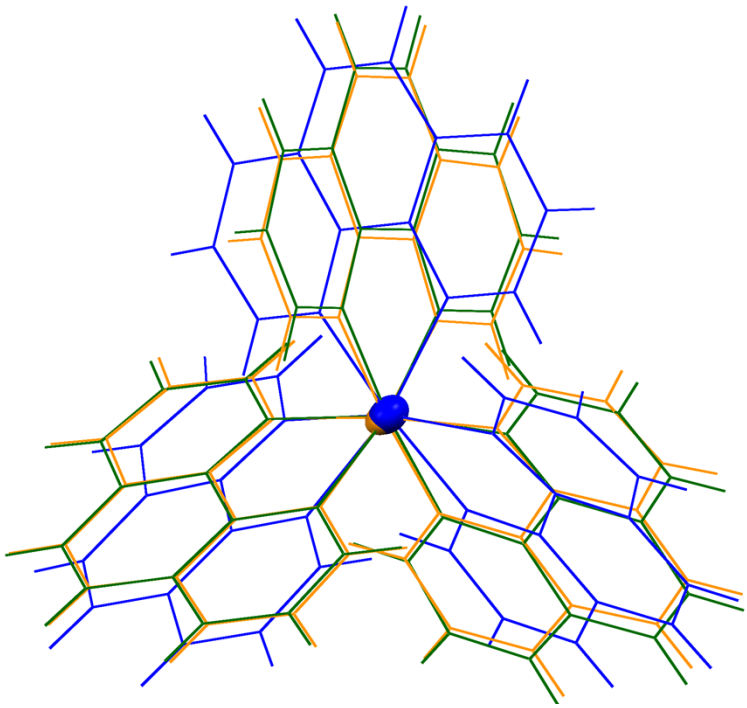

Fig. S2 Complex cations $[M(phen)_3]^{2+}$ overlay in isostructural compounds **1** (orange), **2** (blue) and **3** (green).

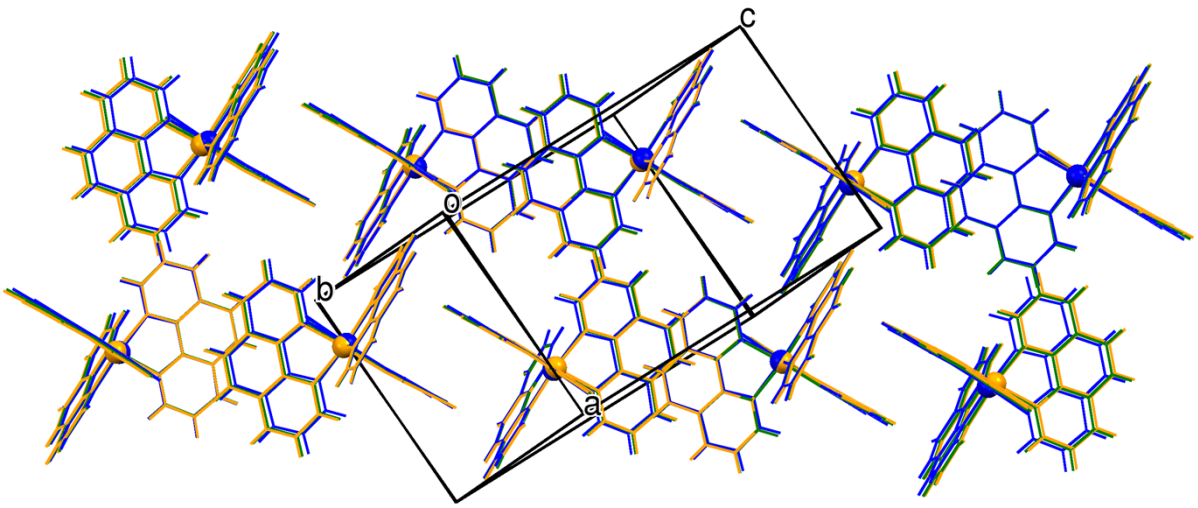

Fig. S3 Overlay of arrangement of the complex cations $[M(phen)_3]^{2+}$ driven by aromatic stacking interactions and $(OFF)(EF)_2$ contacts in isostructural compounds **1** (orange), **2** (blue) and **3** (green).

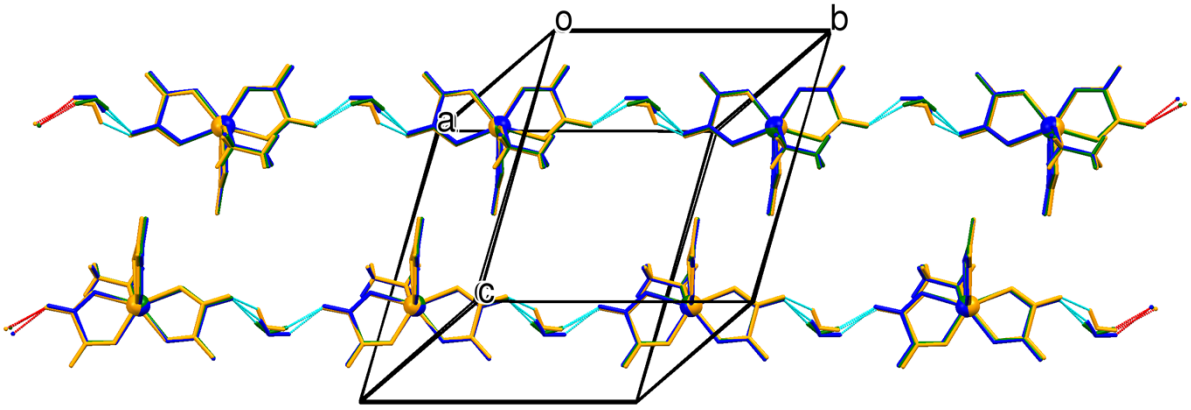

Fig. S4 Overlay of infinite one-dimensional hydrogen-bonding pattern along the *b* axis in the crystal packing of the $[Ta(OC_2H_5)(C_2O_4)_3]^{2-}$ anions and water molecules in isostructural compounds **1** (orange), **2** (blue) and **3** (green).

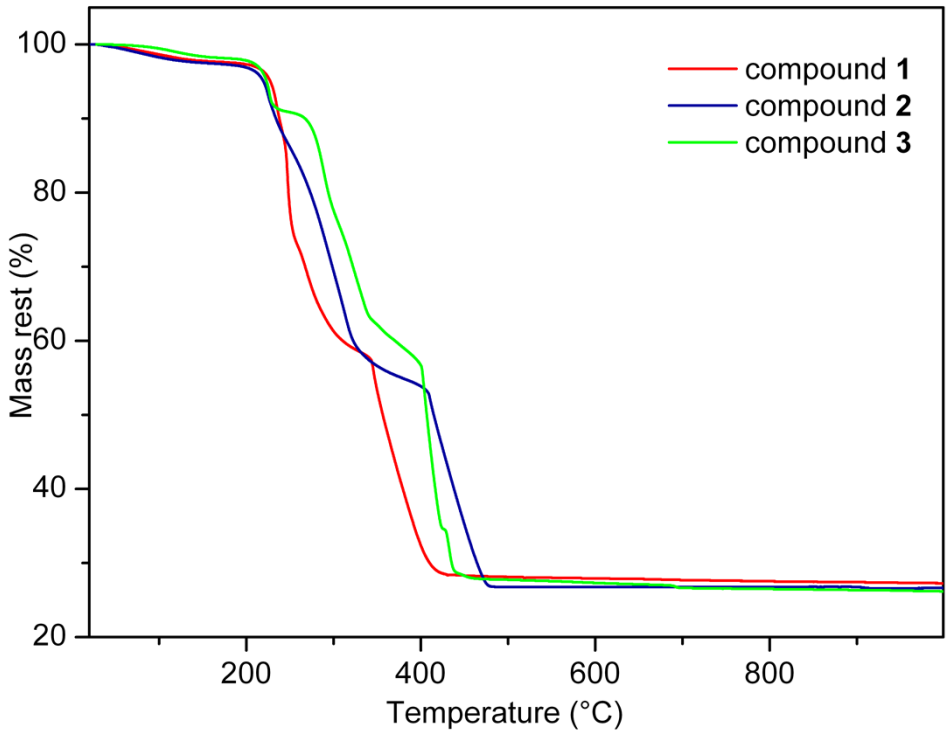

Fig. S5 The TG curves of compounds **1**–**3** measured in the synthetic air.

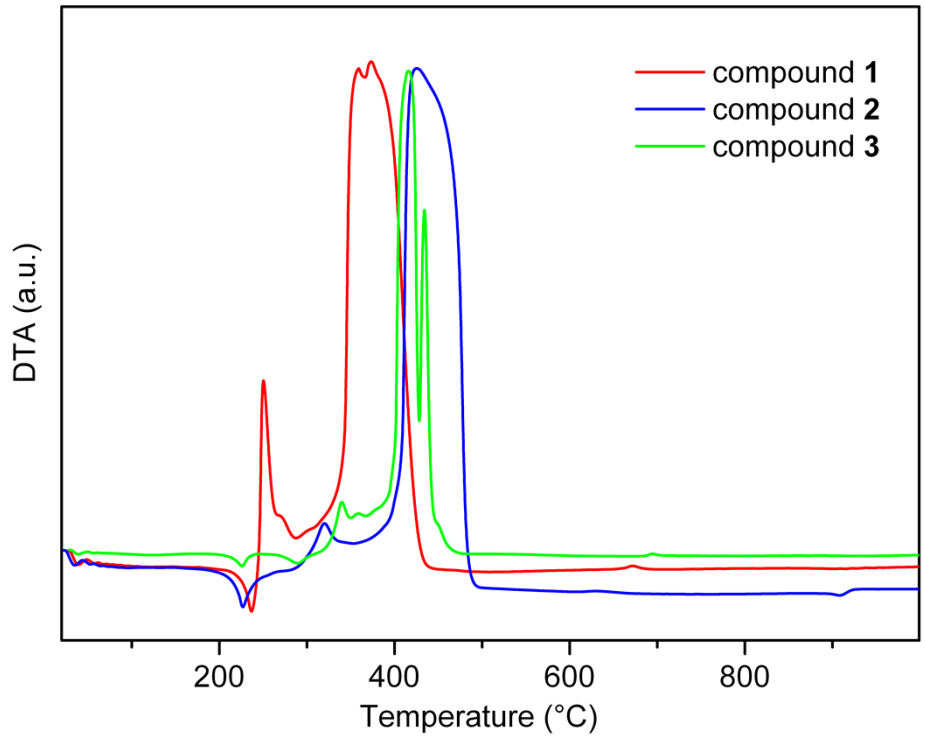

Fig. S6 The DTA curves of compounds **1**–**3** measured in the synthetic air.

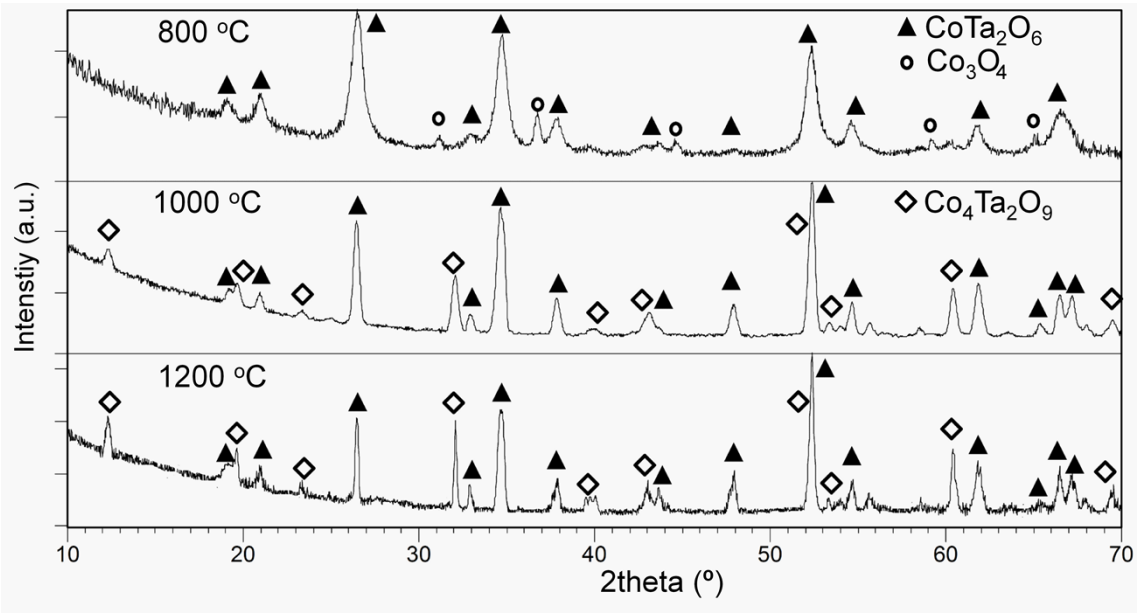

Fig. S7 The X-ray diffraction patterns of samples obtained by heating compound **2** up to 800 1000 and 1200 °C and cooling to room temperature.