Supplementary material

Supramolecular Potential of Vanadium *β*-Diketonate and Picolinate Compounds and The First One-dimensional Oxidovanadium(IV) Complex with *β*-Diketonate Ligand

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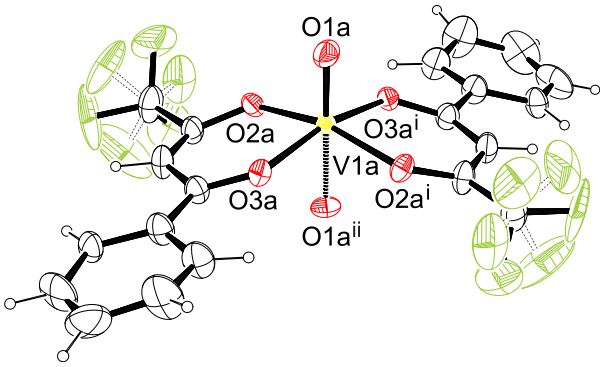

Fig. S1. The molecule of **1b** showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 20% probability level. The disorder of CF_3 groups is indicated by dashed lines, minor part of disordered vanadyl moiety and phenyl ring is omitted for clarity (symmetry codes: (i) $-x, -y, z$; (ii) $-x, y, z - ½$).

Table S1. Selected bond distances and angles for **1b**.

Distance	(Å)		
V1A–O1A	1.54(2)	V1B–O1B	1.54(3)
V1A–O2A	1.970(10)	V1B–O2B	2.007(17)
V1A–O3A	1.992(9)	V1B–O3B	1.984(14)
V1A–O1A^{ii}	2.23(2)	V1B–O1B^{iii}	2.24(3)
Angle	(°)		
O1A–V1A–O1A^{ii}	180.000(1)	O1B–V1B–O1B^{iii}	180.000(4)
O1A–V1A–O2A	98.5(4)	O1B–V1B–O2B	100.3(6)
O1A–V1A–O3A	97.2(4)	O1B–V1B–O3B	101.7(6)
O2A–V1A–O2A^{i}	163.1(8)	O2B–V1B–O2B^{i}	159.4(12)
O2A–V1A–O3A	89.1(5)	O2B–V1B–O3B	88.5(7)
O2A–V1A–O3A^{i}	88.7(5)	O2B–V1B–O3B^{i}	87.4(6)
O3A–V1A–O3A^{i}	165.7(8)	O3B–V1B–O3B^{i}	156.6(12)
O1A^{ii}–V1A–O2A	81.5(4)	O1B^{iii}–V1B–O2B	78.3(6)
O1A^{ii}–V1A–O3A	82.8(4)	O1B^{iii} –V1B–O3B	79.7(6)

Symmetry codes: (i) $-x, -y, z$; (ii) $-x, y, z - ½$; (iii) $-x, y, z + ½$.