substance: V_2O_5
property: band structure: cluster calculations and data

No band structure has been reported. Calculations using the CNDO/2 method have been carried out on clusters $(VO_n)^{5-2n}$, n = 4, 5, 6, where – with reference to Fig. 1 – the n = 6 cluster is shown. The n = 5 cluster is derived from this by removal of $O_1(2)$ to give an approximate square pyramid and in the n = 4 cluster the $O_2(1)$ atom is also removed to leave an approximately tetrahedral VO_4^{3-} ion.

bonds, populations and energies E_B in clusters n = 4, 5, 6
(from [77L])

Bond	n = 6		n = 5		n = 4	
	population	E_B [eV]	population	E_B [eV]	population	E_B [eV]
$V - O_1(1)$	0.438	– 1.319	0.490	– 1.244	0.518	– 1.122
$V - O_1(2)$	0.121	– 0.766	–	–	–	–
$V - O_2(1)$	0.289	– 0.975	0.296	– 0.915	–	–
$V - O_2(2)$	0.350	– 1.118	0.351	– 1.035	0.370	– 0.936
$V - O_2(3)$	0.350	– 1.103	0.351	– 1.035	0.370	– 0.936
$V - O_3$	0.377	– 1.175	0.381	– 1.119	0.420	– 0.963

References:

61B Bachmann, H. G., Ahmed, F. R., Barnes, W. H.: Z. Kristallogr. 115 (1961) 110.
77L Lazukova, N. I., Gubanov, V. A., Mokerov, V. G.: Int. J. Quantum Chem. 12 (1977) 915.

Fig. 1.

V_2O_5. Crystal structure in perspective view [61B].