substance: V_nO_{2n+1}: n ≥ 3
property: crystal structure of V_6O_{13}

Only three oxides have been reported with stoichiometry V_3O_7, V_4O_9 and V_6O_{13}. Of these, V_4O_9 is uncertain and no transport data have been reported for V_3O_7.

High-temperature phase: monoclinic, space group C_{2h}^3 – C2/m, Z = 2 [73S1].

Low-temperature phase: monoclinic, space group C_{2h}^5 – $P2_1/a$ [73S2, 78K].

Crystallographic transition temperature T_{tr} = 151 K↑, 147 K↓ [73S1].

lattice parameters

a	11.921 Å	high-tempera-	variation with temperature: Fig. 1	74D
b	3.6811 Å	ture phase	(refinements given by	
c	10.147 Å	at RT	[74D, 78K, 71W])	
β	100.88°		unit cell: Fig. 2	
a	11.963 Å	low-tempera-		74D
b	3.707 Å	ture phase		
c	10.064 Å	at 120 K		
β	100.96°			

interatomic distances and angles

(distances in Å, angles in °, at 20°C; from [71W])

Two types of structural elements can be distinguished: a single zig-zag string (Fig. 2I) and a double zig-zag ribbon (Fig. 2II) with infinite extension perpendicular to the plane of the paper.

(a) Structure element I, the single zig-zag string

Metal oxygen distances			Bond angles		Bond angles at V(11)	Distances between the oxygen atoms
V(11) –	O(41)	1.766(1)	O(41) – V(11)–	O(11)	179.6(2)	3.830(4)
	O(14) (2×)	1.876(1)	O(41)	O(14) (2×)	101.2(2)	2.815(3)
	O(51)	1.964(5)	O(41)	O(51)	89.0(2)	2.618(4)
	O(61)	1.993(4)	O(41)	O(61)	89.4(2)	2.649(4)
	O(11)	2.064(4)	O(11)	O(14) (2×)	78.8(2)	2.504(5)
			O(11)	O(51)	90.7(2)	2.865(6)
			O(11)	O(61)	91.0(2)	2.894(6)
			O(14)	O(14)	157.6(3)	3.680(1)
			O(14)	O(51) (2×)	90.2(2)	2.721(4)
			O(14)	O(61) (2×)	90.1(2)	2.740(4)
			O(51)	O(61)	178.4(2)	3.958(6)

Metal-metal separations
(< 3.50 Å)
V(11) – V (14) 3.047(2)

(b) Structure element II, the double zig-zag ribbon

Metal oxygen distances			Bond angles		Bond angles at V(21) and V(31)	Distances between the oxygen atoms
V(21) –	O(51)	1.655(5)	O(5l) – V(21) –	O(32)	102.3(2)	2.925(6)
	O(71)	1.761(4)	O(51)	O(23) (2×)	97.4(2)	2.677(4)
	O(23) (2×)	1.902(1)	O(51)	O(71)	104.9(3)	2.708(6)
	O(32)	2.084(4)	O(51)	O(72)	176.5(2)	3.930(6)
	O(72)	2.277(5)	O(32)	O(23) (2×)	76.1(2)	2.462(4)
V(31) –	O(61)	1.641(4)	O(32)	O(71)	152.8(2)	3.738(6)
	O(33) (2×)	1.919(1)	O(32)	O(72)	74.1(2)	2.633(6)
	O(72)	1.928(4)	O(23)	O(23)	150.7(3)	3.680(1)
	O(22)	1.981(4)	O(23)	O(71) (2×)	100.2(2)	2.810(4)
	O(32)	2.261(4)	O(23)	O(72) (2×)	81.8(2)	2.751(4)
			O(71)	O(72)	78.6(3)	2.589(9)
			O(61) – V(31) –	O(32)	176.8(2)	3.901(6)
			O(61)	O(33) (2×)	103.4(2)	2.800(4)

Valence balance gives V(1): + 4.16 *e*, V(2): + 4.60 *e*, V(3): + 4.34 *e* [74D]. The only crystallographic change below 147 K is that V(1) shifts by 0.14 Å along the *b*-axis, destroying the mirror plane [78K].

References:

71W Wilhelmi, K. A., Waltersson, K., Kihlborg, L.: Acta Chem. Scand. 25 (1971) 2671.

73S1 Saeki, M., Kimizuka, N., Ishii, M., Kawada, I., Ichinose, A., Nakahira, M.: J. Cryst. Growth 18 (1973) 101.

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Fig. 1.

V_6O_{13}. Lattice parameters vs. temperature [74D].

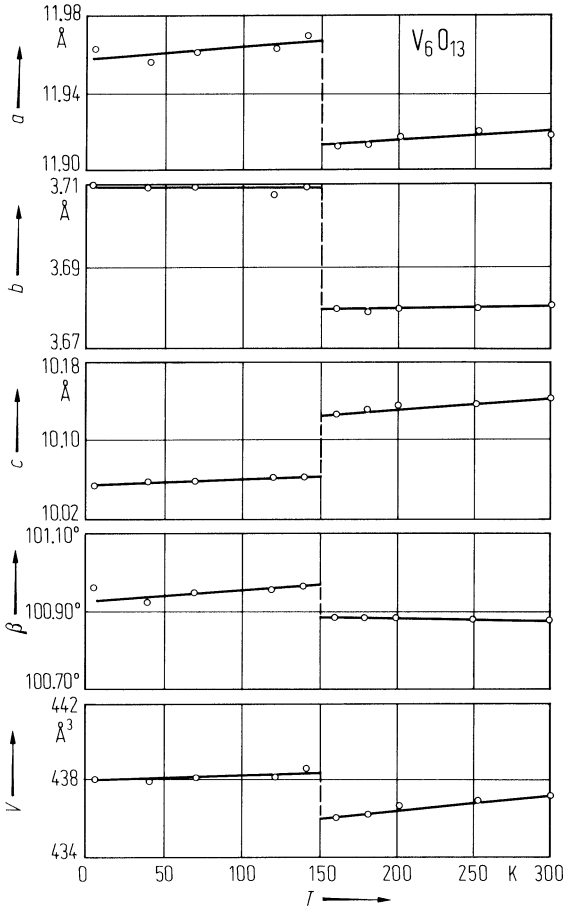

Fig. 2.

V_6O_{13}. Crystal structure projected on (010). The two types of structure elements that can be distinguished are shown. The numbering of atoms refers to the tables [71W]. Dashed line in upper figure shows unit cell. Open circles: V atom above *ac* plane, full circles: V atom below *ac* plane.