substance: V_nO_{2n-1}: n ≥ 3
property: crystal structure of V_5O_9

Space group C_i^1 –A $\bar{1}$, *Z* = 2.

lattice parameters

a	5.472(1 Å	RT	variation with temperature: see	74M
b	7.003(1) Å		Fig. 1; a clear transition is	
c	8.727(1) Å		seen at ca. 130 K	
α	97.49°			
β	112.40°			
γ	109.01°			

A view of the RT structure looking down the triclinic *a*-axis is seen in Fig. 2. There are two independent strings V(5)–V(3)–V(1)–V(3)–V(5) and V(6)–V(4)–V(2)–V(4)–V(6). Below the transition, charge ordering occurs, but is not complete, and there is no crystallographic evidence for any particular pairing scheme. The estimated change in partial charges at the transition is (in units of *e*): V(1) 3.8–4.1. V(2) 3.7–3.5, V(3) 3.6–3.8, V(4) 3.5–3.2, V(5) 3.6–3.8, V(6) 3.5–3.3.

References:

74M Marezio, M., Dernier, P. D., McWhan, D. B., Kachi, S.: J. Solid State Chem. 11 (1974) 301.

Fig. 1.

V_5O_9. Lattice parameters vs. temperature [74M].

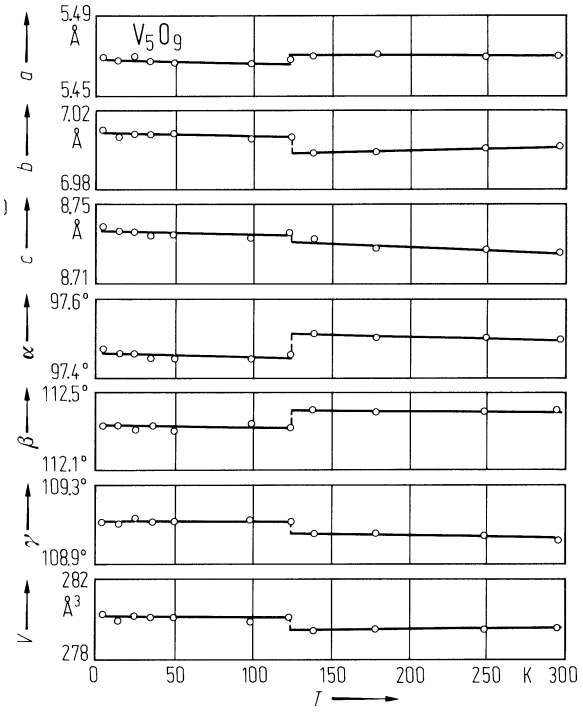

Fig. 2.

V_5O_9. Projection of the structure down the triclinic axis at RT [74M].