

**substance:**  $V_nO_{2n-1}$ :  $n \geq 3$

**property:** crystal structure of  $V_4O_7$

Space group:  $C_1^1 - A\bar{1}$ ,  $Z = 4$ .

**lattice parameters**

$a$	5.509(1) Å	RT	variation with temperature: see	78H,
$b$	7.008(2) Å		Fig. 1 (transition at $\approx 240$ K);	73M,
$c$	12.256(2) Å		positional parameters are given	72H
$\alpha$	95.10(2)°		for three temperatures in [73K]	
$\beta$	95.17(1)°			
$\gamma$	109.25(2)°			
$V$	441.33 Å <sup>3</sup>			

The structure is a shear phase closely related to  $Ti_4O_7$  (q.v.) and there are two independent strings of vanadium atoms V(4)–V(2)–V(2)–V(4) and V(3)–V(1)–V(1)–V(3). At room temperature, the partial charges are (in units of  $e$ ) 3.48–3.35–3.34–3.48 and 3.64–3.53–3.53–3.64 with a much shorter V(1)–V(1) distance than V(2)–V(2), V(3)–V(1) or V(2)–V(4). At ca. 240 K a transition is seen, in which charge differentiation takes place to give charge distributions of 3.11–3.22–3.22–3.11 and 3.84–3.83–3.83–3.84 at 200 K and 3.09–3.24–3.24–3.09 and 3.84–3.83–3.83–3.84 at 120 K. The main structural alteration is the development of two short V(2)–V(4) distances below the transition temperature.

## References:

- 70M     Marezio, M., McWhan, D. B., Dernier, P. D., Remeika, J. P.: Mater. Res. Bull. 5 (1970) 1015.
- 72H     Horiuchi, H., Tokonami, M., Morimoto, N., Nagasawa, K.: Acta Crystallogr. B28 (1972) 1404.
- 73K     Kachi, S., Kosuge, K., Okinaka, H.: J. Solid State Chem. 6 (1973) 258.
- 73M     Marezio, M., McWhan, D. B., Dernier, P. D., Remeika, J. P.: J. Solid State Chem. 6 (1973) 419.
- 78H     Hodeau, J. L., Marezio, M.: J. Solid State Chem. 23 (1978) 253.

**Fig. 1.**

$V_4O_7$ . Lattice parameters vs. temperature [70M].

