

**Data Table 5 V<sub>2</sub>O<sub>5</sub> (14)**

---

Orthorhombic, space group *Pmmn*, No. 59;  $a = 11.51$ ,  $b = 3.56$ ,  $c = 4.37$  Å;  
 $Z = 2$ ,  $V = 179$  Å<sup>3</sup>

*Atomic Positions*

V in 4(*f*):  $x, 0, z; \bar{x}, 0, z; \frac{1}{2} - x, \frac{1}{2}, \bar{z}; \frac{1}{2} + x, \frac{1}{2}, \bar{z}; x = 0.1487, z = 0.1086$   
O(1) in 4(*f*):  $x = 0.1460, z = 0.4713$   
O(2) in 4(*f*):  $x = 0.3191, z = -0.0026$   
O(3) in 2(*a*):  $0, 0, z; \frac{1}{2}, \frac{1}{2}, \bar{z}; z = -0.0031$