

**substance: V<sub>2</sub>O<sub>5</sub>**

**property: interatomic distances and angles, thermal expansion**

**interatomic distances and angles**

Values in parentheses give the estimated standard deviation [61B]. Atoms are labelled as in Fig. 1.

|   |            |
|---|------------|
| V – O <sub>1</sub> (1)                  | 1.585(4) Å |
| V – O <sub>1</sub> (2)                  | 2.785(5) Å |
| V – O <sub>2</sub> (1)                  | 2.021(3) Å |
| V – O <sub>2</sub> (2)                  | 1.878(2) Å |
| V – O <sub>2</sub> (3)                  | 1.878(2) Å |
| V – O <sub>3</sub>                      | 1.780(2) Å |
| O <sub>1</sub> (1) – O <sub>2</sub> (1) | 2.873(5) Å |
| O <sub>1</sub> (1) – O <sub>2</sub> (2) | 2.744(4) Å |
| O <sub>1</sub> (1) – O <sub>2</sub> (3) | 2.744(4) Å |
| O <sub>1</sub> (1) – O <sub>3</sub>     | 2.668(5) Å |
| O <sub>2</sub> (1) – O <sub>2</sub> (2) | 2.388(3) Å |
| O <sub>2</sub> (1) – O <sub>2</sub> (3) | 2.388(3) Å |
| O <sub>2</sub> (1) – O <sub>3</sub>     | 3.673(4) Å |
| O <sub>1</sub> (2) – O <sub>2</sub> (3) | 3.563(3) Å |
| O <sub>3</sub> (2) – O <sub>3</sub>     | 2.740(3) Å |
| O <sub>3</sub> (3) – O <sub>3</sub>     | 2.740(3) Å |
| O <sub>1</sub> (2) – O <sub>2</sub> (1) | 3.042(5) Å |
| O <sub>1</sub> (2) – O <sub>2</sub> (2) | 2.954(4) Å |
| O <sub>1</sub> (2) – O <sub>2</sub> (3) | 2.954(4) Å |
| O <sub>1</sub> (2) – O <sub>3</sub>     | 2.846(5) Å |

angles:

|   |           |
|---|-----------|
| O <sub>1</sub> (1) – V – O <sub>2</sub> (1) | 105.0(2)° |
| O <sub>1</sub> (1) – V – O <sub>2</sub> (2) | 104.5(3)° |
| O <sub>1</sub> (1) – V – O <sub>2</sub> (3) | 104.5(3)° |
| O <sub>1</sub> (1) – V – O <sub>3</sub>     | 104.8(3)° |
| O <sub>2</sub> (1) – V – O <sub>2</sub> (2) | 75.5(2)°  |
| O <sub>2</sub> (1) – V – O <sub>2</sub> (3) | 75.5(2)°  |
| O <sub>2</sub> (1) – V – O <sub>3</sub>     | 150.1(2)° |
| O <sub>2</sub> (2) – V – O <sub>2</sub> (3) | 143.1(2)° |
| O <sub>2</sub> (2) – V – O <sub>3</sub>     | 97.0(2)°  |
| O <sub>2</sub> (3) – V – O <sub>3</sub>     | 97.0(2)°  |

**coefficients of linear thermal expansion**

|            |                                     |                                  |     |
|------------|-------------------------------------|----------------------------------|-----|
| $\alpha_a$ | $2.0 \cdot 10^{-6} \text{ K}^{-1}$  | $T = 25 \dots 600^\circ\text{C}$ | 67K |
| $\alpha_b$ | $55.4 \cdot 10^{-6} \text{ K}^{-1}$ |                                  |     |
| $\alpha_c$ | $8.0 \cdot 10^{-6} \text{ K}^{-1}$  |                                  |     |

**References:**

- 61B     Bachmann, H. G., Ahmed, F. R., Barnes, W. H.: Z. Kristallogr. 115 (1961) 110.  
67K     Kennedy, T. N., Hakim, R., McKenzie, J. D.: Mater. Res. Bull. 2 (1967) 193.

**Fig. 1.**

$\text{V}_2\text{O}_5$ . Crystal structure in perspective view [61B].

