

**substance: WO<sub>3</sub>**

**property: phonon wavenumbers, Debye temperature**

**wavenumbers of Raman active phonons**

at RT (in cm<sup>-1</sup>)

( <i>v/c</i> ) <sub>R</sub>	277, 330, 722, 810	intense peaks in Raman spectra	69B
	275, 297, 328, 352, 718, 808		69R
	275, 330, 719, 508		75S2
	275, 718, 807		69M
	224, 327, 349, 378, 406, 418, 445, 574, 642	weaker peaks in Raman spectra	69M
	71,83,135	lines below 200 cm <sup>-1</sup> . These low frequency phonons show marked changes with temperature, Fig. 1	69R
	33, 60, 73, 93, 133		75S2

**wavenumbers of IR active phonons**

at RT (in cm<sup>-1</sup>)

( <i>v/c</i> ) <sub>IR</sub>	765, 825, 920	intense bands in IR spectra	75S2
	775, 535, 900		75K
	768, 825, 920		69R
	745, 815, 920		69M
	226, 252, 280, 290, 307, 322, 340, 360, 386	lower frequency bands	75K
	230, 285, 310, 335, 370		75S1
	375, 390		70O
	218, 241, 275, 295.5, 314, 328, 350.5, 378		76A

**Debye temperature**

Θ <sub>D</sub>	350(15) K	<i>T</i> = 1...55 K	heat capacity	74B
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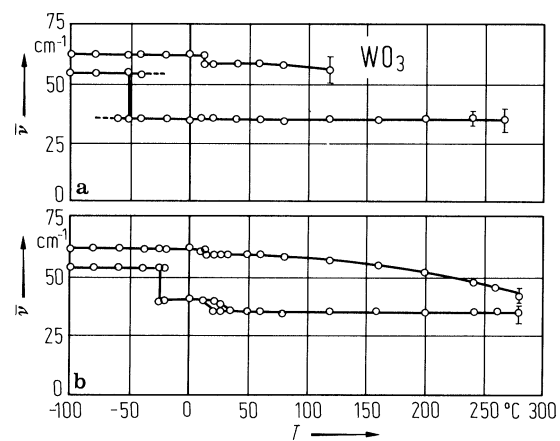
Below – 50°C WO<sub>3</sub> is piezoelectric (Fig. 2). Antiferroelectric grain boundaries are evident at low temperatures [51M, 70B, 72S, 76S].

## References:

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**Fig. 1.**

WO<sub>3</sub>. Wavenumber of low-frequency optical phonons vs. temperature. (a) and (b) refer to the monoclinic room temperature form and a triclinic form also stable at room temperature [75S1].



**Fig. 2.**

$\alpha$ - $\text{WO}_3$ . Average piezoelectric coefficient vs. temperature [75S1].

