No. 22A-3 $TlGaSe_2$, Thallium gallium selenide

(M = 432.03)

1a Ferroelectricity in $TlGaSe_2$ was found by Hochheimer et al. in 1988. 88Hoc

b

phase	III	II	I	
state	F	P	P	88Hoc
crystal system	monoclinic	monoclinic	monoclinic [a])	[a]) 78Mul
space group	Cc– C_s^4		C2/c– C_{2h}^6 [a])	
Θ [K]	110		120	88Hoc

Phase transitions: see 84Ali
$\rho = 6.40 \cdot 10^3$ kg m^{-3}, $\rho_X = 6.42 \cdot 10^3$ kg m^{-3}. 78Mul
$T_{melt} \approx 780$ °C. 75Isa
Color: deep red. 75Isa
Cleavage plane: (001). 88Hoc

2a Synthesis and crystal growth by Stockbarger method: see 75Isa
Bridgman method in evacuated quartz ampoules: see 84Ali, 82Hen

3a Unit cell parameters: a = 10.772(3) Å, b = 10.771(5) Å, c = 15.636(8) Å, β = 100.6(3)° at RT. 78Mul, 82Hen

b Z = 16. 78Mul
Crystal structure at RT: Table 22A-3-001.
$TlGaSe_2$ crystallizes with a layer structure with two anion layers perpendicular to $\boldsymbol{c}^*$. 78Mul
For crystal model, atomic coordinates, interatomic distances: see 78Mul

5a Dielectric constant vs. temperature: Fig. 22A-3-001, Fig. 22A-3-002, Fig. 22A-3-003, Fig. 22A-3-004.
See also 84Ali, 91Sar
Curie-Weiss law holds: $\Theta_f \approx 107$ K, $C \approx 5.4 \cdot 10^3$ K. 88Hoc
Dielectric dispersion: Fig. 22A-3-005, Fig. 22A-3-006.

c Spontaneous polarization vs. temperature: Fig. 22A-3-007.

d Pyroelectric coefficient: Fig. 22A-3-008.

6 Heat capacity anomalies were observed at 108.9 K and 118.4 K. 84Abd
Debye temperature Θ_D = 97K (estimated at about 7 K). 84Abd
C_p data suggest additional phase transitions at 246 K and about 101 K. 86All

9a Optically positive (slightly biaxial) $2V$ = 4.2° at 20 °C. 84Ali
Optical transmission vs. λ: see 75Isa
Infrared active modes: see 83Gas
Optical absorption and Urbach edge: Fig. 22A-3-009.
Absorption spectra at 1.8 K in the range 2.0...2.5 eV (exciton spectra): see 85Abu
See also 85All
See also subsection 11 below.

10a Raman spectra: Scattering intensity vs. frequency shift.
Fig. 22A-3-010, Fig. 22A-3-011.
Frequency shift vs. temperature: Fig. 22A-3-012.

	See also	75Isa, 83Gas, 89Bur
	Pressure dependence of the Raman active modes (300 K and 110 K): see	82Hen
b	Brillouin scattering: Fig. 22A-3-013, Fig. 22A-3-014.	
11	Photoconductivity: see For exciton behaviour, see also subsection 9a above.	83Abd