61 $NH_2CH_2COOH \cdot AgNO_3$

61A Pure compound

No. 61A-1 $NH_2CH_2COOH \cdot AgNO_3$, Glycine silver nitrate

(M = 244.94)

1a Ferroelectricity in $NH_2CH_2COOH \cdot AgNO_3$ was discovered by Pepinsky et al. in 1957. 57Pep

b

phase	II	I
state	F	P
crystal system		monoclinic
space group		$P2_1/a - C_{2h}^5$
Θ [°C]	–55	

57Pep

Θ = –43 °C for $ND_2CH_2COOD \cdot AgNO_3$. 77Ges
P_s || [010]. 57Pep
T_{melt} = 145 °C. 72Moh
$\rho = 2.79 \cdot 10^3$ kg m^{-3}, $\rho_X = 2.806 \cdot 10^3$ kg m^{-3}. 72Moh
Transparent, colorless but usually brown as a result of illumination by light. 64Mit
Cleavage plane: (010). 69Tod

2a Crystal growth: cooling and evaporation methods from aqueous solution. 57Pep
Slow introduction of ethyl alcohol vapor into the saturated aqueous solution. 57Pep
Crystal form: Fig. 61A-1-001.

3a Unit cell parameters: a = 5.451 Å, b = 19.493 Å, c = 5.541 Å, β = 100.20(25)° in phase I. 72Moh

b Z = 4 in phase I. 72Moh
Crystal structure: Table 61A-1-001, Table 61A-1-002, Table 61A-1-003, Table 61A-1-004, Table 61A-1-005; Fig. 61A-1-002, Fig. 61A-1-003, Fig. 61A-1-004, Fig. 61A-1-005, Fig. 61A-1-006.

4 Lattice distortions: Fig. 61A-1-007, Fig. 61A-1-008.

5a Dielectric constants: Fig. 61A-1-009, Fig. 61A-1-010, Fig. 61A-1-011.
Effect of hydrostatic pressure on partially deuterated crystal: see 77Ges
$\kappa_b = C/(T - \Theta_p)$, $T > \Theta_f$, C = 446 K, Θ_p = –55 °C. 64Mit
Curie-Weiss constant changes with hydrostatic pressure as $C = C_0(1 + \beta p)$, 77Ges
C_0 = 860(40) K, $\beta = -0.17(2) \cdot 10^{-8}$ Pa^{-1} in the range $p < 1.8 \cdot 10^8$ Pa.
Phase diagram in regard to p: Fig. 61A-1-012.
Phase diagram for partially deuterated crystal: see 77Ges

b Nonlinear dielectric properties: $\xi = 5.2 \cdot 10^{14}$ V m^5 C^{-3}. 64Mit

c Spontaneous polarization and coercive field: Fig. 61A-1-013, 61A-1-014.

7b Electrostrictive constants: $\Delta a/a\, P_s^2 = Q_{12} \approx -18$ C^{-2} m^4, $\Delta b/b\, P_s^2 = Q_{22} \approx 36$ C^{-2} m^4, 64Mit
$\Delta c/c\, P_s^2 \approx 300$ C^{-2} m^4, $\Delta\beta/\beta P_s^2 \approx 220$ C^{-2} m^4 at –100 °C.

13a NMR: Fig. 61A-1-015.

Table 61A-1-001. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. Fractional coordinates.

		Fractional coordinates			Fractional coordinates
Ag	*x*	0.1450(4)	O(5)	*x*	–0.095(4)
	y	0.01631(10)		*y*	0.1360(10)
	z	–0.1855(4)		*z*	–0.038(4)
O(1)	*x*	0.166(3)	N(1)	*x*	0.689(4)
	y	0.0430(9)		*y*	0.1589(11)
	z	0.401(3)		*z*	0.403(5)
O(2)	*x*	0.412(3)	N(2)	*x*	0.047(4)
	y	0.0645(9)		*y*	0.1884(10)
	z	0.126(3)		*z*	–0.030(4)
O(3)	*x*	0.151(3)	C(1)	*x*	0.355(5)
	y	0.2074(10)		*y*	0.0710(12)
	z	0.180(4)		*z*	0.333(5)
O(4)	*x*	0.103(5)	C(2)	*x*	0.516(5)
	y	0.2124(13)		*y*	0.1166(15)
	z	–0.222(5)		*z*	0.524(6)

Table 61A-1-002. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. Temperature parameter B_{ij} is defined by Eq. (a) in Introduction.

Ag	B_{11}	0.0275(6)	O(3)	B_{11}	0.035(7)	N(1)	B_{11}	0.030(7)
	B_{22}	0.00293(4)		B_{22}	0.0030(5)		B_{22}	0.0021(6)
	B_{33}	0.0314(6)		B_{33}	0.049(8)		B_{33}	0.046(9)
	B_{12}	–0.0061(3)		B_{12}	0.004(3)		B_{12}	–0.003(3)
	B_{13}	0.0041(11)		B_{13}	–0.022(12)		B_{13}	–0.010(14)
	B_{23}	–0.0035(3)		B_{23}	–0.006(3)		B_{23}	0.005(4)
O(1)	B_{11}	0.029(6)	O(4)	B_{11}	0.043(11)	N(2)	B_{11}	0.024(7)
	B_{22}	0.0032(5)		B_{22}	0.0053(9)		B_{22}	0.0020(5)
	B_{33}	0.032(7)		B_{33}	0.052(10)		B_{33}	0.052(10)
	B_{12}	–0.003(3)		B_{12}	–0.002(4)		B_{12}	0.001(3)
	B_{13}	–0.006(11)		B_{13}	–0.001(18)		B_{13}	–0.005(15)
	B_{23}	–0.004(3)		B_{23}	0.002(5)		B_{23}	–0.002(3)
O(2)	B_{11}	0.021(5)	O(5)	B_{11}	0.040(8)	C(1)	B_{11}	0.036(9)
	B_{22}	0.0027(5)		B_{22}	0.0021(5)		B_{22}	0.0013(5)
	B_{33}	0.032(6)		B_{33}	0.054(9)		B_{33}	0.033(10)
	B_{12}	–0.001(3)		B_{12}	–0.003(4)		B_{12}	–0.004(3)
	B_{13}	–0.004(9)		B_{13}	–0.018(15)		B_{13}	–0.036(14)
	B_{23}	–0.003(3)		B_{23}	–0.003(4)		B_{23}	–0.001(4)
						C(2)	B_{11}	0.028(9)
							B_{22}	0.023(8)
							B_{33}	0.034(13)
							B_{12}	–0.007(4)
							B_{13}	–0.014(19)
							B_{23}	–0.006(5)

Table 61A-1-003. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. Interatomic distances around Ag atoms.

	Distance [Å]
Ag–O (1) (–*x*, –*y*, –*z*)	2.22(2)
Ag–O (2)	2.25(2)
Ag–O (1) (*x*, *y*, *z* – 1)	2.37(2)
Ag–O (2) (–*x* + 1, –*y*, –*z*)	2.85(2)
Ag–O (5)	2.86(2)
Ag–Ag (–*x*, –*y*, –*z*)	2.877(6)

Table 61A-1-004. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. Interatomic angles around Ag atoms.

	Angle [deg]
O(1)(–*x*, –*y*, –*z*)–Ag–O(2)	163.1(7)
O(5)–Ag–O(2)(–*x* + 1, –*y*, –*z*)	146.7(5)
O(1)(*x*, *y*, *z* – 1)–Ag–Ag(–*x*, –*y*, –*z*)	149.9(4)
O(1)(–*x*, –*y*, –*z*)–Ag–O(5)	103.5(6)
O(5)–Ag–O(2)	73.0(6)
O(2)–Ag–O(2)(–*x* + 1, –*y*, –*z*)	73.9(6)
O(2)(–*x* + 1, –*y*, –*z*)–Ag–O(1)(–*x*, –*y*, –*z*)	109.0(6)
O(1)(*x*, *y*, *z* – 1)–Ag–O(5)	101.5(6)
O(5)–Ag–Ag(–*x*, –*y*, –*z*)	68.9(4)
Ag(–*x*, –*y*, –*z*)–Ag–O(2)(–*x* + 1, –*y*, –*z*)	110.9(4)
O(2)(–*x* + 1, –*y*, –*z*)–Ag–O(1)(*x*, *y*, *z* – 1)	92.8(5)
O(1)(–*x*, –*y*, –*z*)–Ag–O(1)(*x*, *y*, *z* – 1)	76.0(7)
O(1)(*x*, *y*, *z* – 1)–Ag–O(2)	120.9(6)
O(2)–Ag–Ag(–*x*, –*y*, –*z*)	84.7(4)
Ag(–*x*, –*y*, –*z*)–Ag–O(1)(–*x*, –*y*, –*z*)	79.1(5)
C(1)–O(2)–Ag	120.8(15)
O(1)–C(1)–O(2)	124.9(23)
Ag(–*x*, –*y*, –*z*)–O(1)–C(1)	130.0(17)

Table 61A-1-005. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. Interatomic distances and angles in NO_3 group.

Distance [Å]		Angle [deg]	
N(2)–O(3)	1.26(3)	O(3)–N(2)–O(4)	123(2)
N(2)–O(4)	1.25(4)	O(3)–N(2)–O(5)	116(2)
N(2)–O(5)	1.28(3)	O(4)–N(2)–O(5)	120(2)

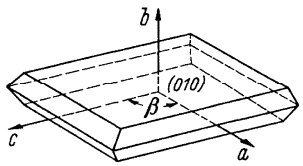

Fig. 61A-1-001. $NH_2CH_2COOH \cdot AgNO_3$. Crystal form [64Mit].

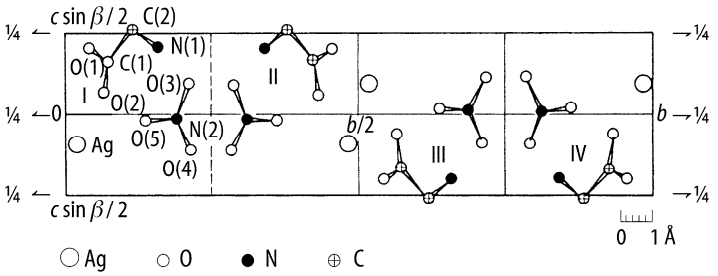

Fig. 61A-1-002. $NH_2CH_2COOH \cdot AgNO_3$. Structure of phase I [72Moh]. View along the *a* axis. The Roman numerals indicate the equivalent positions, and the relevant symmetry operations are as follows: I: *x*, *y*, *z*; II: 1/2 + *x*, 1/2 – *y*, *z*; III: 1/2 – *x*, 1/2 + *y*, –*z*; IV: –*x*, –*y* + 1, –*z*.

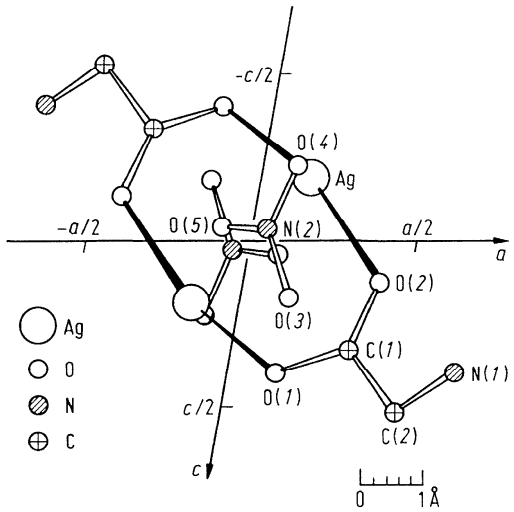

Fig. 61A-1-003. $NH_2CH_2COOH \cdot AgNO_3$. Strucure of phase I [72Moh]. View along the *b* axis, showing the existence of glycine dimers bridged by silver atoms.

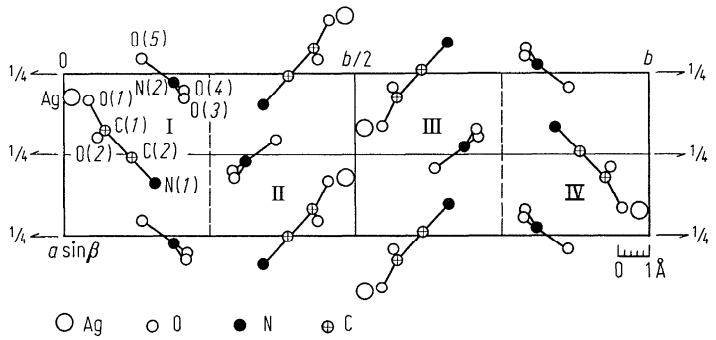

Fig. 61A-1-004. $NH_2CH_2COOH \cdot AgNO_3$. Strucure of phase I [72Moh]. View along the *c* axis. See Fig. 61A-1-002 for Roman numerals.

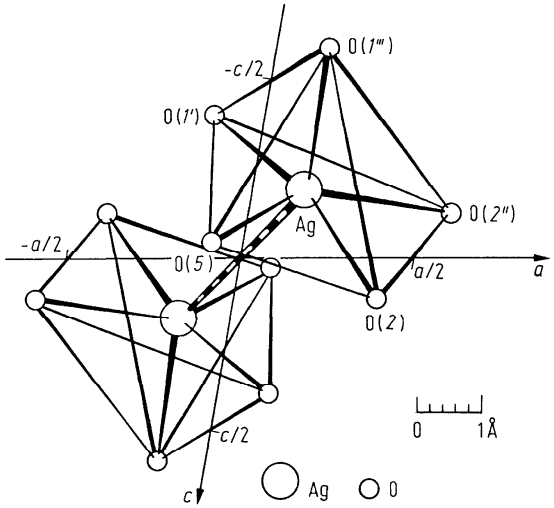

Fig. 61A-1-005. $NH_2CH_2COOH \cdot AgNO_3$. Strucure of phase I [72Moh]. Surroundings of the inversion center at (0, 0, 0). The Ag-Ag bond is represented by thick, partially shaded lines. The labelled atoms have the following coordinates: O(2), O(5), Ag: (x, y, z); O(1′): ($-x$, $-y$, $-z$); O(2″): ($-x + 1$, $-y$, $-z$); O(1‴): (x, y, $z - 1$).

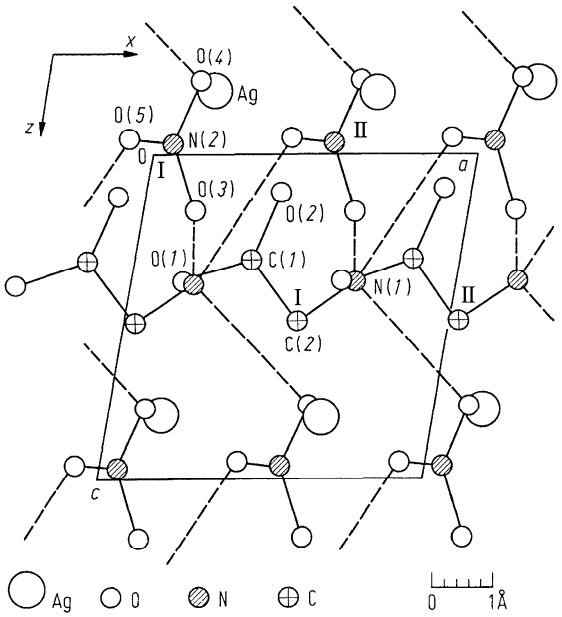

Fig. 61A-1-006. $NH_2CH_2COOH \cdot AgNO_3$. Strucure of phase I [72Moh]. Hydrogen bondings (broken lines) viewed along the *b* axis. See Fig. 61A-1-002 for I and II.

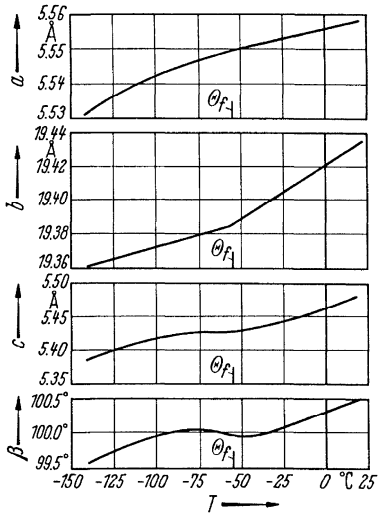

Fig. 61A-1-007. $NH_2CH_2COOH \cdot AgNO_3$. Lattice parameters vs. *T* [64Mit].

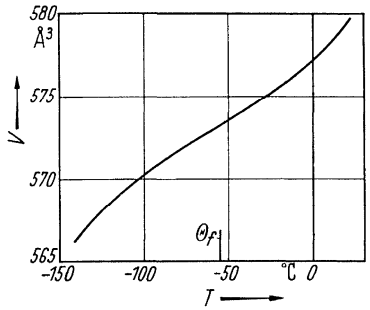

Fig. 61A-1-008. $NH_2CH_2COOH \cdot AgNO_3$. V vs. T [64Mit]. V: unit cell volume.

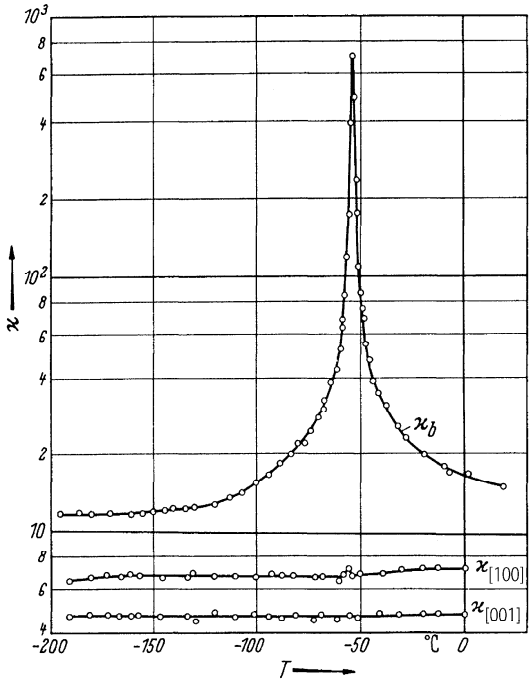

Fig. 61A-1-009. $NH_2CH_2COOH \cdot AgNO_3$. $\varkappa_{[100]}$, $\varkappa_b$, $\varkappa_{[001]}$ vs. T [64Mit]. $f = 10$ kHz.

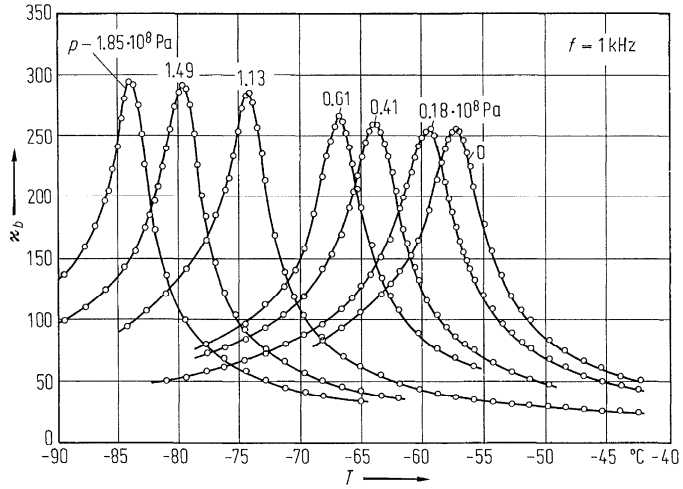

Fig. 61A-1-010. $NH_2CH_2COOH \cdot AgNO_3$. κ_b vs. T [77Ges]. Parameter: p.

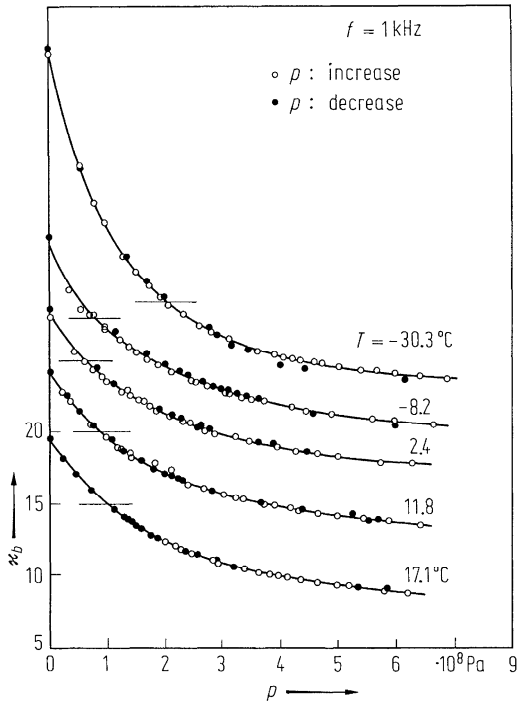

Fig. 61A-1-011. $NH_2CH_2COOH \cdot AgNO_3$. κ_b vs. p [77Ges]. Parameter: T. Thin horizontal lines show the level of $\kappa_b = 15$.

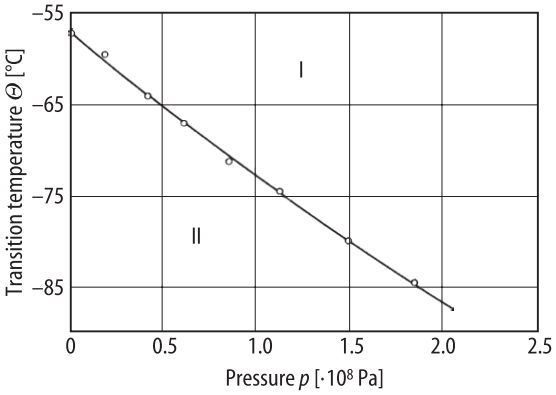

Fig. 61A-1-012. $NH_2CH_2COOH \cdot AgNO_3$. Θ vs. p [77Ges].

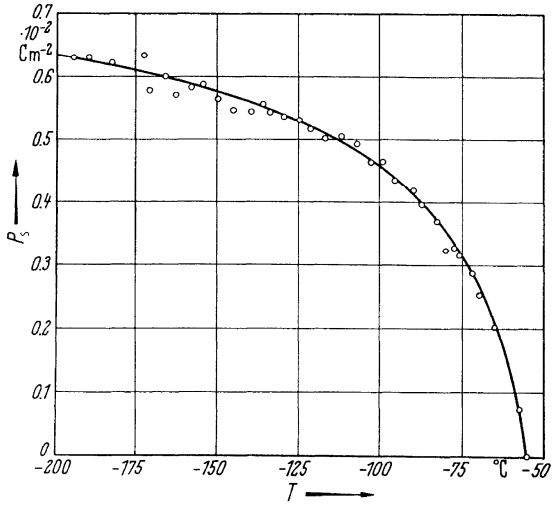

Fig. 61A-1-013. $NH_2CH_2COOH \cdot AgNO_3$. P_s vs. T [64Mit].

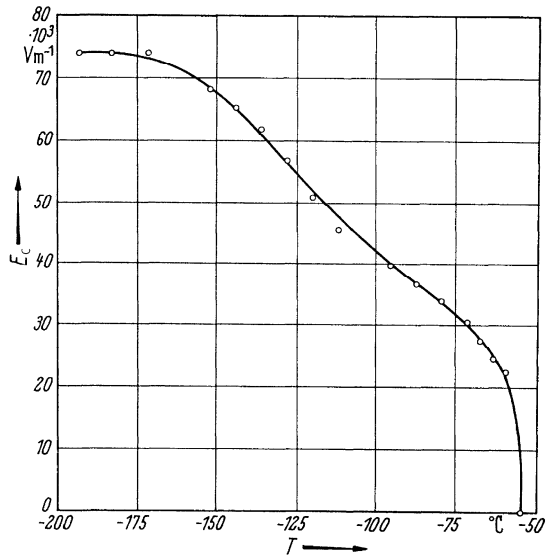

Fig. 61A-1-014. $NH_2CH_2COOH \cdot AgNO_3$. E_c vs. T [57Pep].

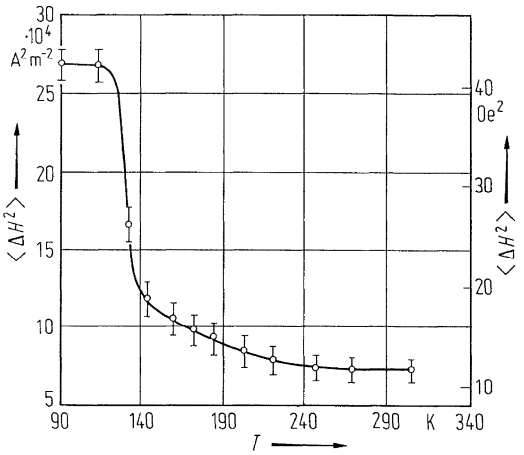

Fig. 61A-1-015. $NH_2CH_2COOH \cdot AgNO_3$. $\langle \Delta H^2 \rangle$ of proton vs. T [66Eas]. $\langle \Delta H^2 \rangle$: second moment of magnetic resonance curve.

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