70 $3C_6H_4(OH)_2 \cdot CH_3OH$

70A Pure compound

No. 70A-1 $3C_6H_4(OH)_2 \cdot CH_3OH$, β-Quinol-methanol clathrate

(M = 362.38)

1a	Reversal of pyroelectric polarity by poling was observed in $3C_6H_4(OH)_2 \cdot CH_3OH$ by Murakami et al. in 1990.			90Mur
b	phase	II	I	90Mur
	state	F		
	crystal system		trigonal	
	space group		$R\bar{3} - C_{3i}^2$	
	Θ [K]	63.7		
	The structure of β-quinol contains cavities approximately 4 Å in diameter, there being one cavity of each three quinol molecules. The methanol molecule is trapped in the cavity.			48Pal
	P_s || [001] of phase I.			90Mur
	Transparent, colorless.			90Mur
2a	Crystal growth: slow evaporation from the methanol solution of $C_6H_4(OH)_2$.			90Mur
3a	Unit cell parameters: a = 16.625 Å, c = 5.566 Å at RT.			90Mur
b	Z = 3 in phase I.			90Mur
	Crystal structure of $3C_6H_4(OH)_2 \cdot xCH_3OH$ (x = 0.887): see			82Mak
5a	Dielectric constant: Fig. 70A-1-001, Fig. 70A-1-002; see also			53Dry, 79Rip
c	Spontaneous polarization: Fig. 70A-1-003.			
6a	Heat capacity: Fig. 70A-1-004; see also			67Mat
9a	Far infrared spectrum: see			73Fuk
13a	NMR: Fig. 70A-1-005, Fig. 70A-1-006; see also			79Rip

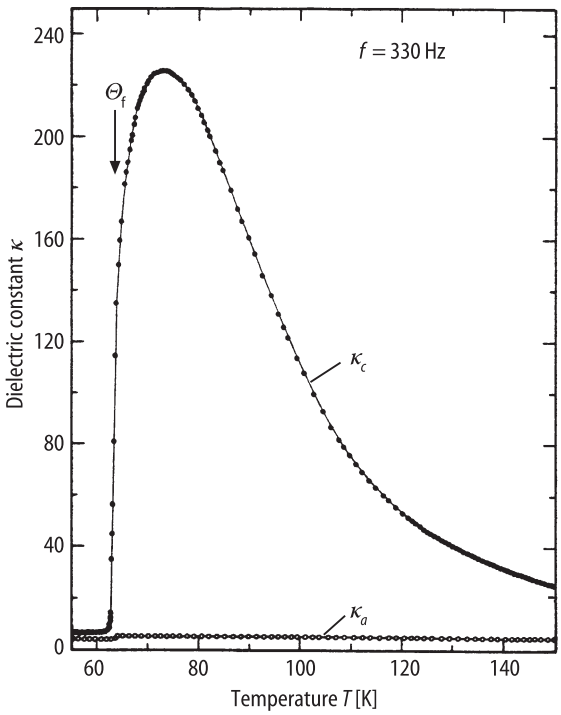

Fig. 70A-1-001. $3C_6H_4(OH)_2 \cdot CH_3OH$. κ_a, κ_c vs. T [90Mur].

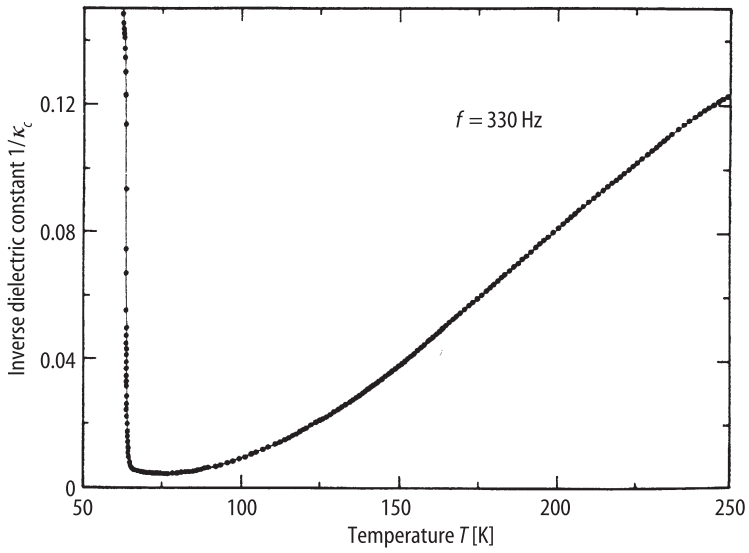

Fig. 70A-1-002. $3C_6H_4(OH)_2 \cdot CH_3OH$. κ_c^{-1} vs. T [90Mur].

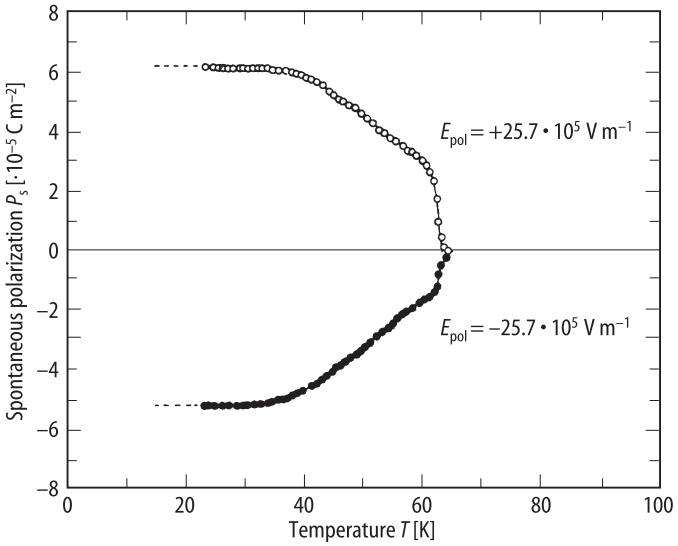

Fig. 70A-1-003. $3C_6H_4(OH)_2 \cdot CH_3OH$. P_s vs. T [90Mur]. Obtained by pyroelectric charge measurement along the c axis. E_{pol}: poling field.

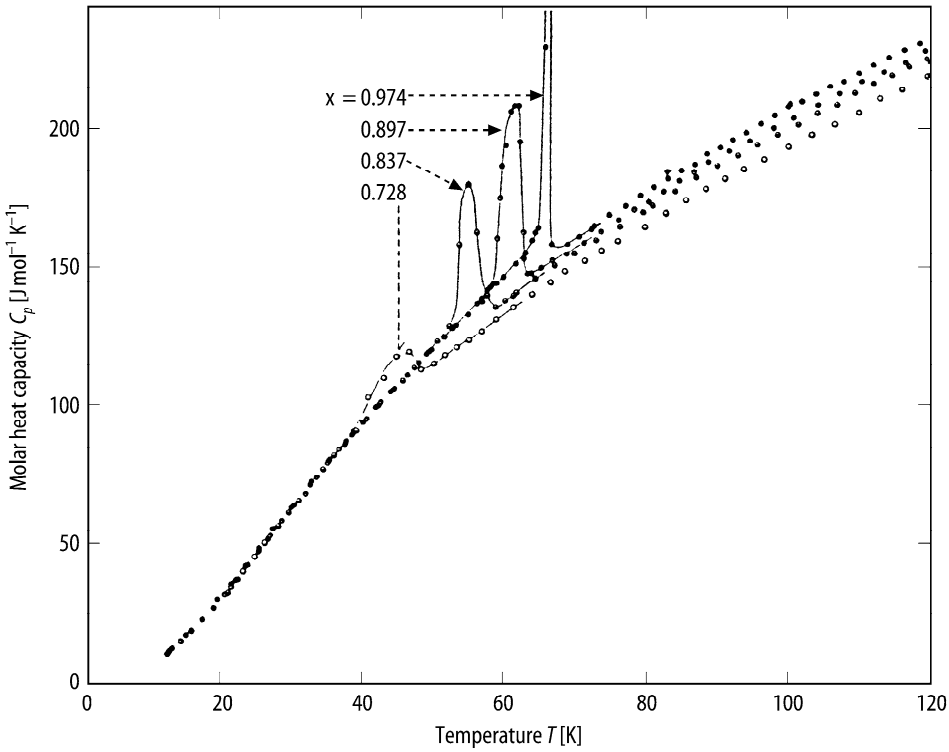

Fig. 70A-1-004. $3C_6H_4(OH)_2 \cdot xCH_3OH$. C_p vs. T [70Mat]. C_p: molar heat capacity at constant pressure. Parameter: x.

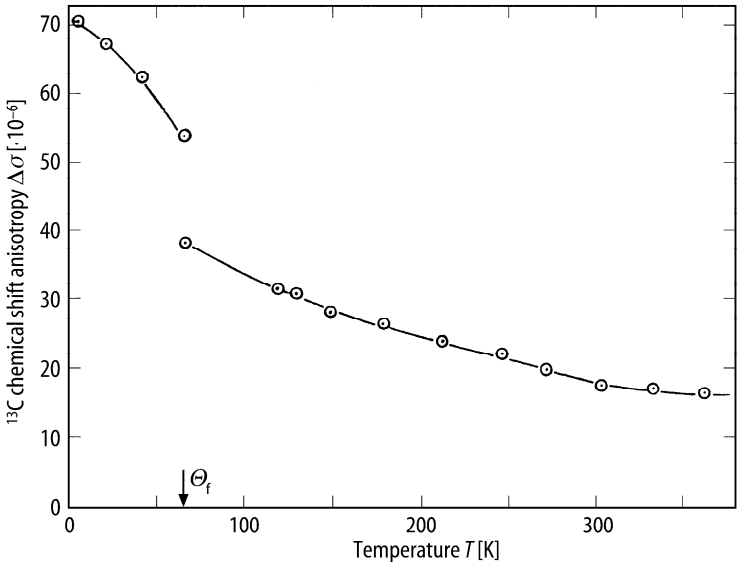

Fig. 70A-1-005. $3C_6H_4(OH)_2 \cdot CH_3OH$. $\Delta\sigma$ vs. T [82Mat]. $\Delta\sigma$: ^{13}C chemical shift anisotropy.

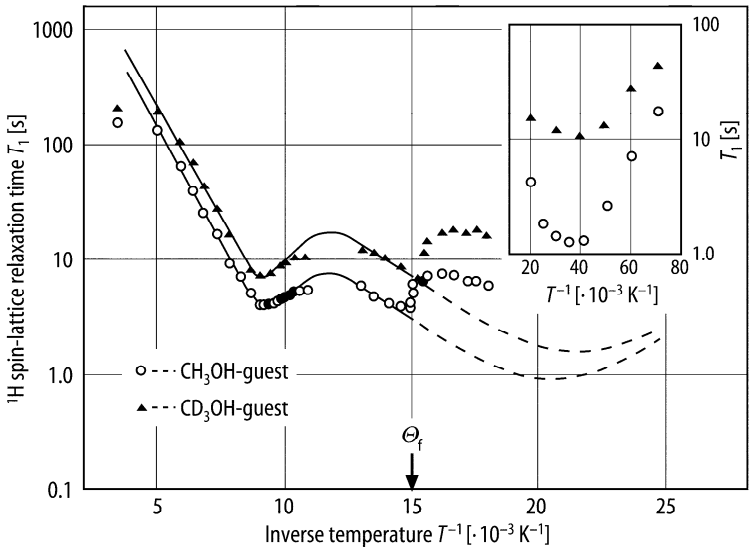

Fig. 70A-1-006. $3C_6H_4(OH)_2 \cdot CH_3OH$. T_1 vs. T^{-1} [82Mat]. T_1: ^{1}H spin-lattice relaxation times with CH_3OH and CD_3OH trapped as the guest. The solid lines show the theoretical fits obtained by assuming the six-site reorientation model. The broken lines show theoretical curves in the fictitious case in which the phase transition and the methyl tunneling are absent.

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