Supporting Information

Facile Resolution of Racemic Terbutaline and A Study of Molecular Recognition through Chiral Supramolecules Based on Enantiodifferentiating Self-Assembly

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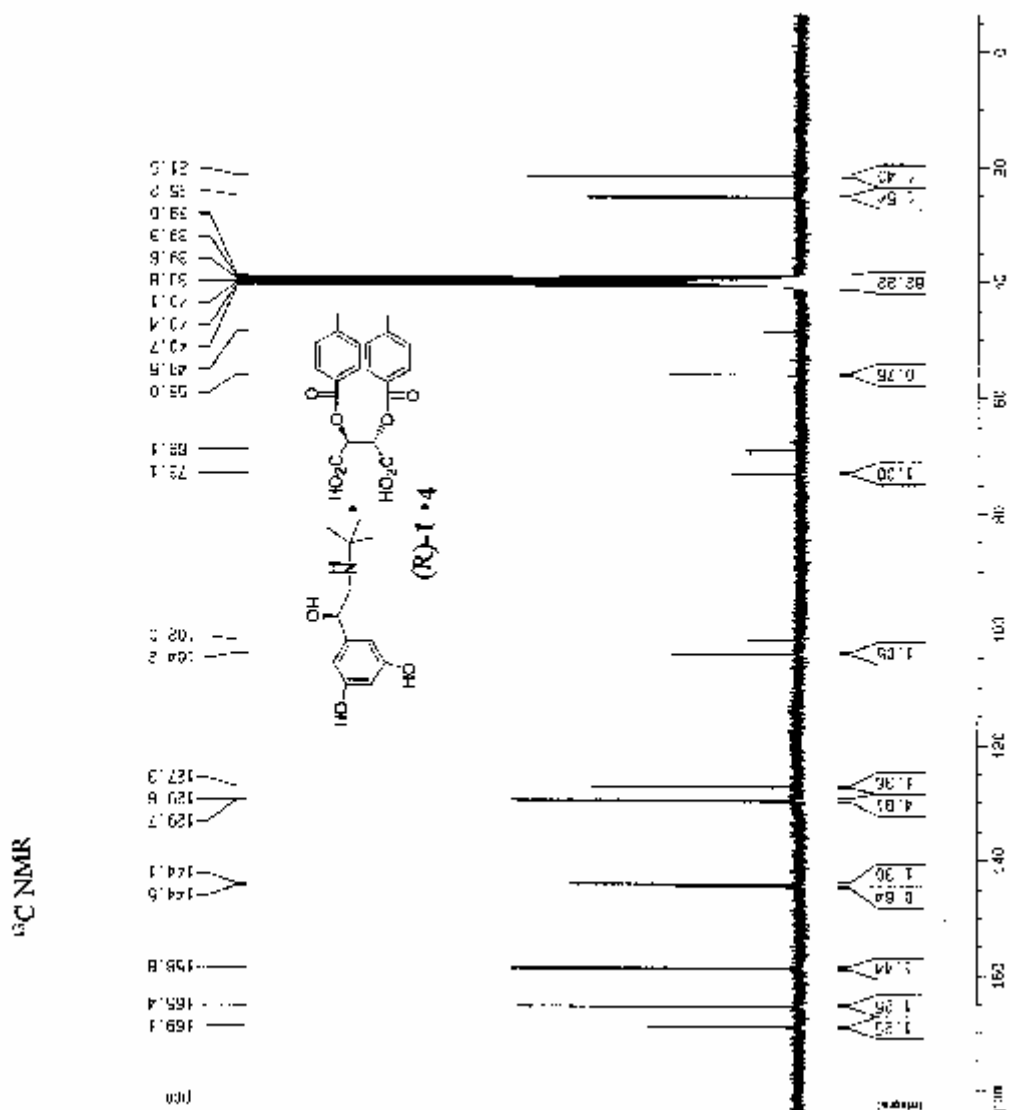1) ^{1}H and ^{13}C NMR analyses of (*R*)-1.4 and (*S*)-1.4

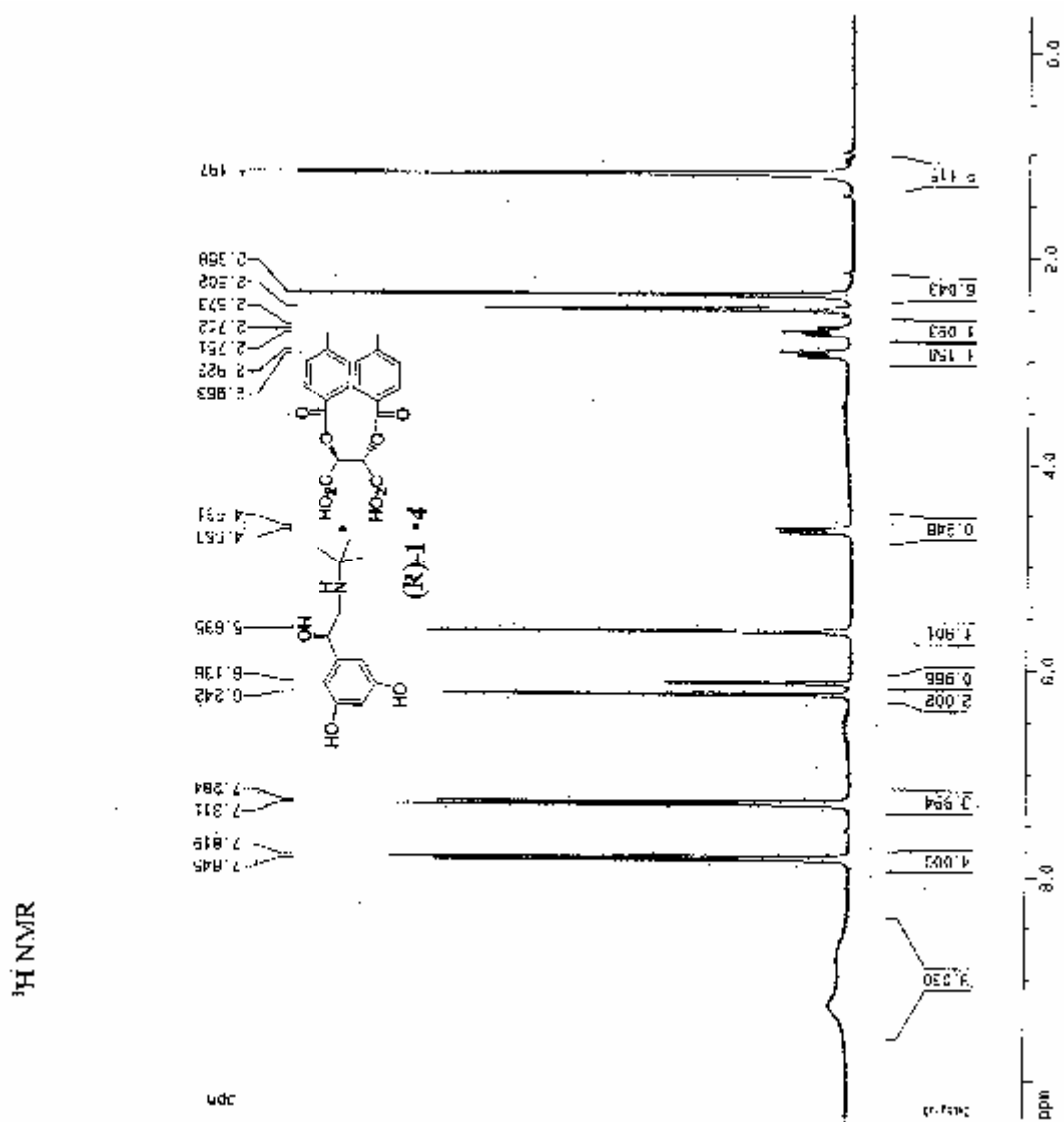**Figure S1.** ^{13}C-NMR spectrum of (*R*)-terbutaline (**1**) and *D*-DTTA (**4**)

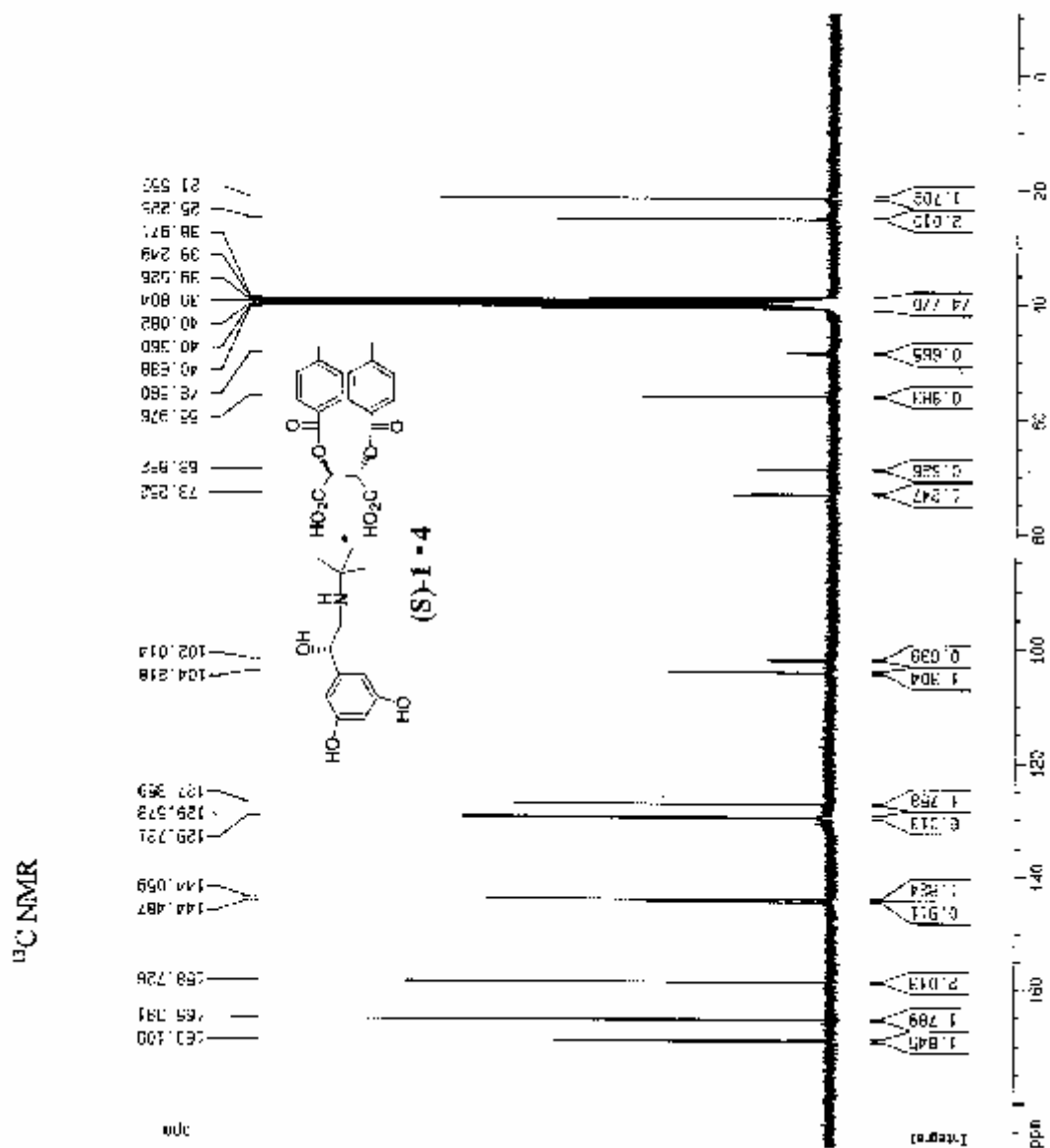**Figure S2.** ¹H-NMR spectrum of (*R*)-terbutaline (**1**) and *D*-DTTA (**4**)

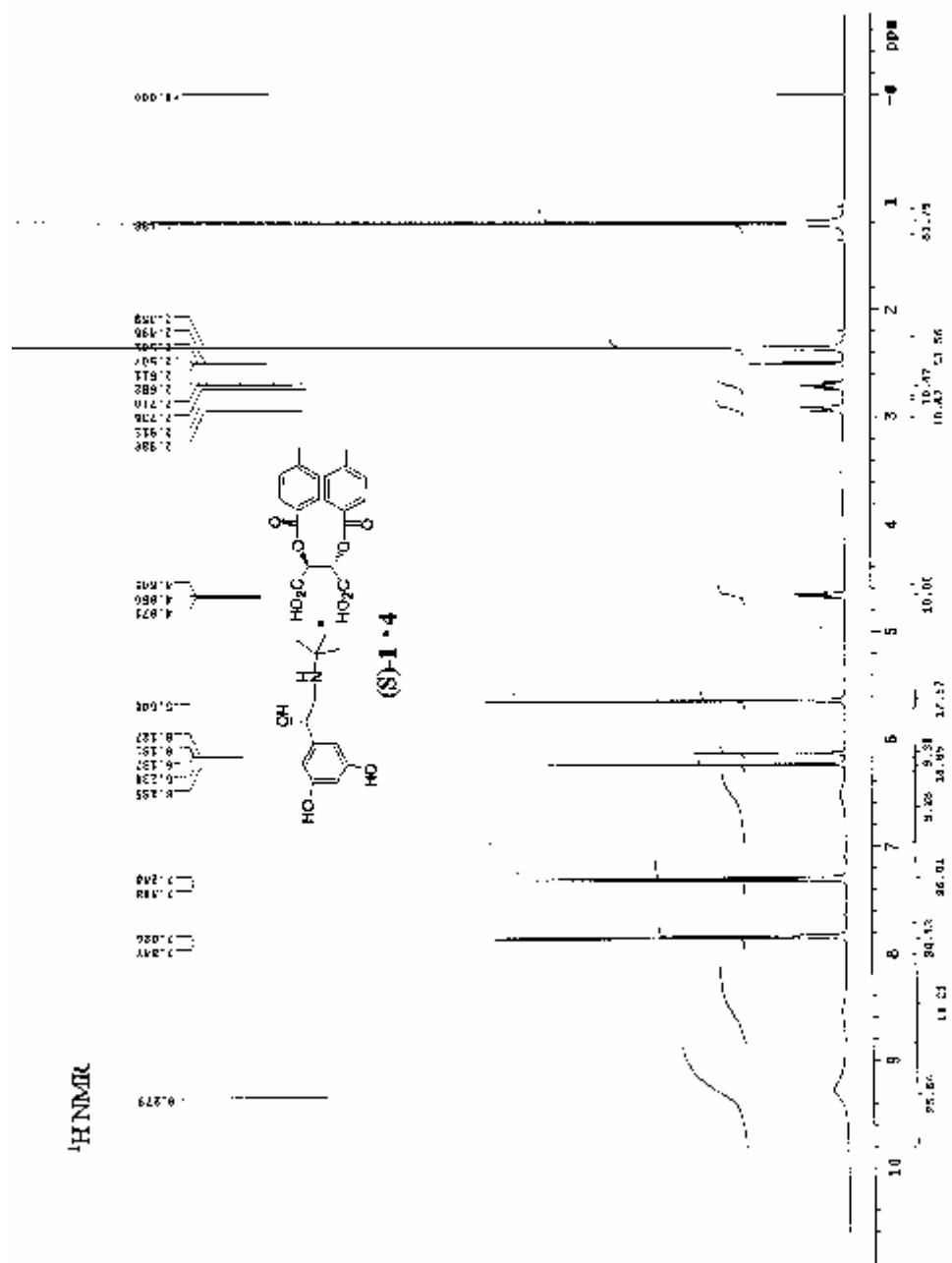**Figure S3.** ^{13}C-NMR spectrum of (*S*)-terbutaline (**1**) and *D*-DTTA (**4**)

Figure S4. ^{1}H-NMR spectrum of (*S*)-terbutaline (**1**) and *D*-DTTA (**4**)

2) ORTEP views and stacking structures of crystals 5, 7 and 8

A

B

C

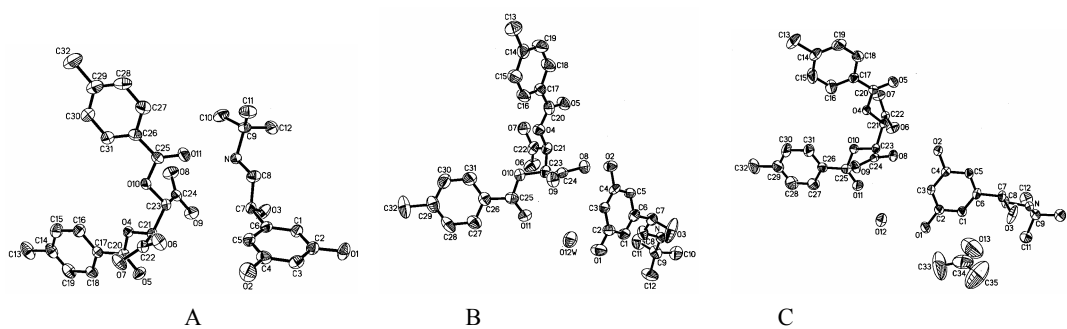**Figure S5.** ORTEP views of the molecular structure of **5** (A), **7** (B) and **8** (C).

A
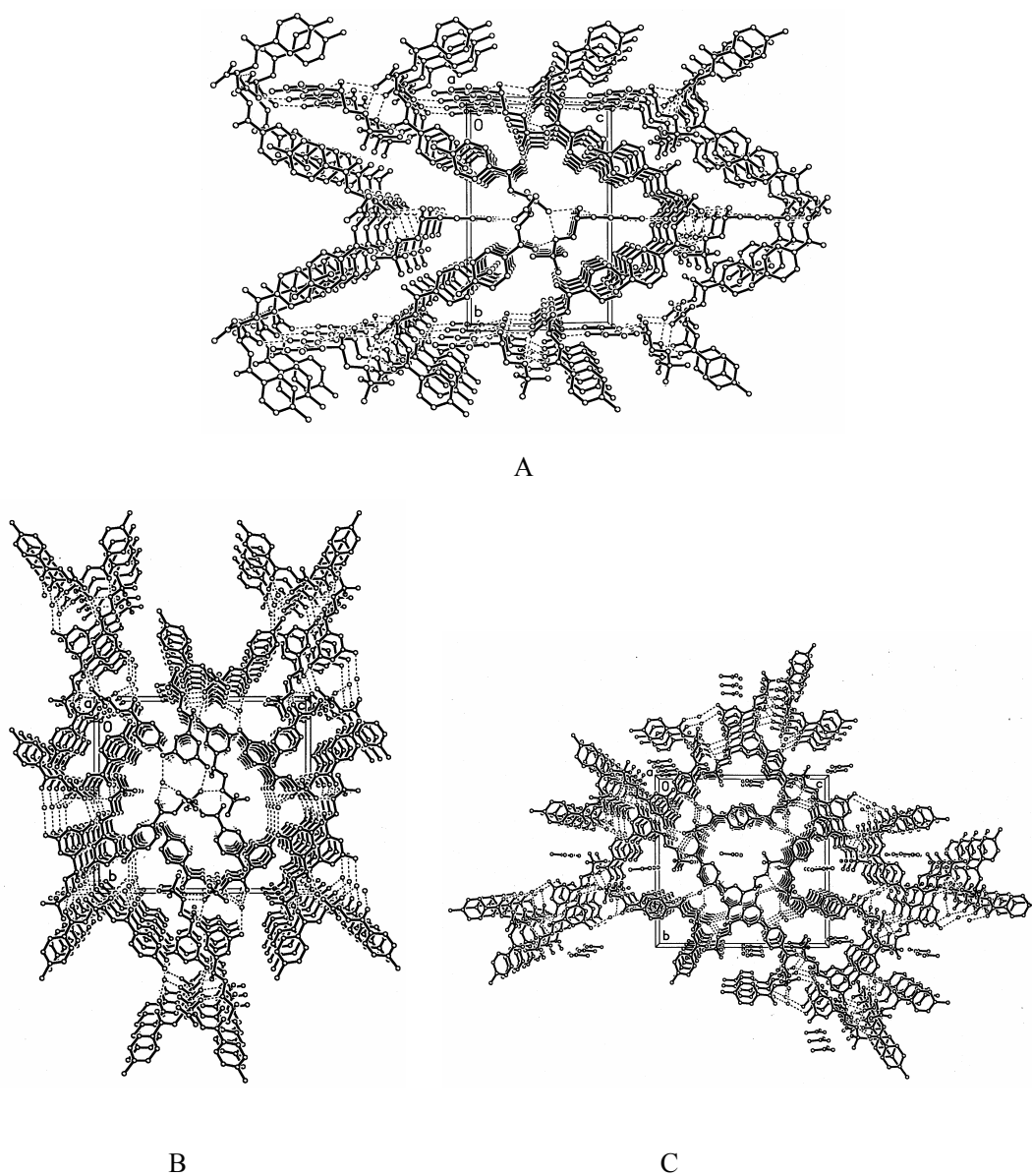
B   C

Figure S6. Stacking structures of crystals **5** (A), **7** (B) and **8** (C) (top view down the *a* axis). All H-bonds are represented by dotted lined.

3) DSC and TG analyses of the more- and less-soluble salts
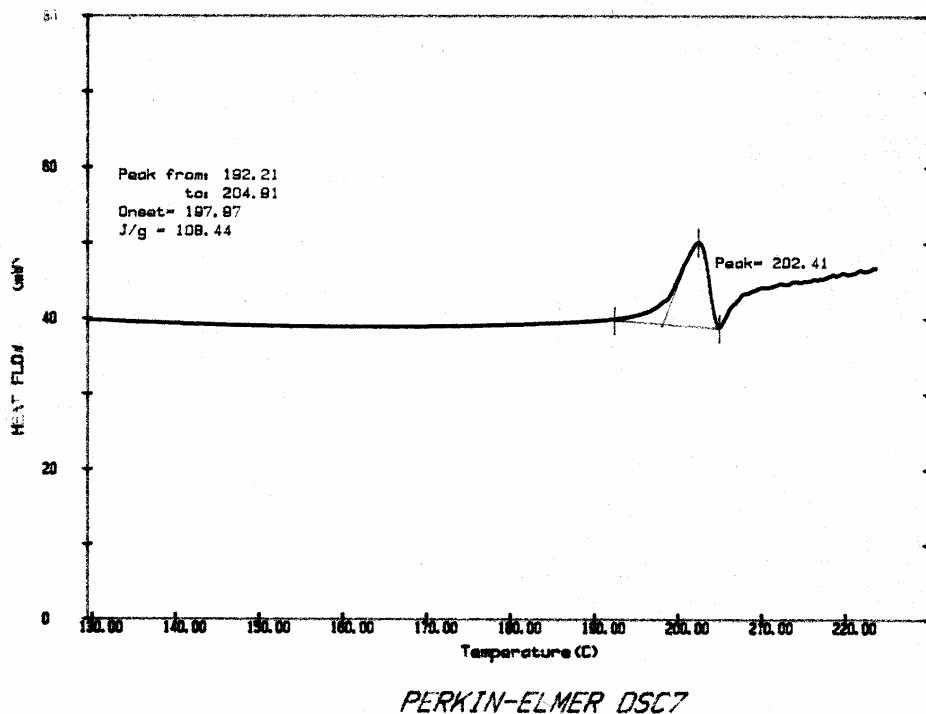
A) For more-soluble salt

Peak from: 192.21
to: 204.81
Onset= 197.87
J/g = 108.44

Peak= 202.41

HEAT FLOW (mW)

Temperature (C)

PERKIN-ELMER DSC7

Figure S7. DSC analysis of the more-soluble salt. $\Delta H_{fus.} = 108.44 \times 611/1000 = 66.2$ KJ/mol

X = 99.270

222.8381

From: 187.33 C
To: 235.83 C
Onset at: 222.83

From: 186.83 C
To: 360.15 C
% Change = 69.599

X = 29.670

WEIGHT (%)

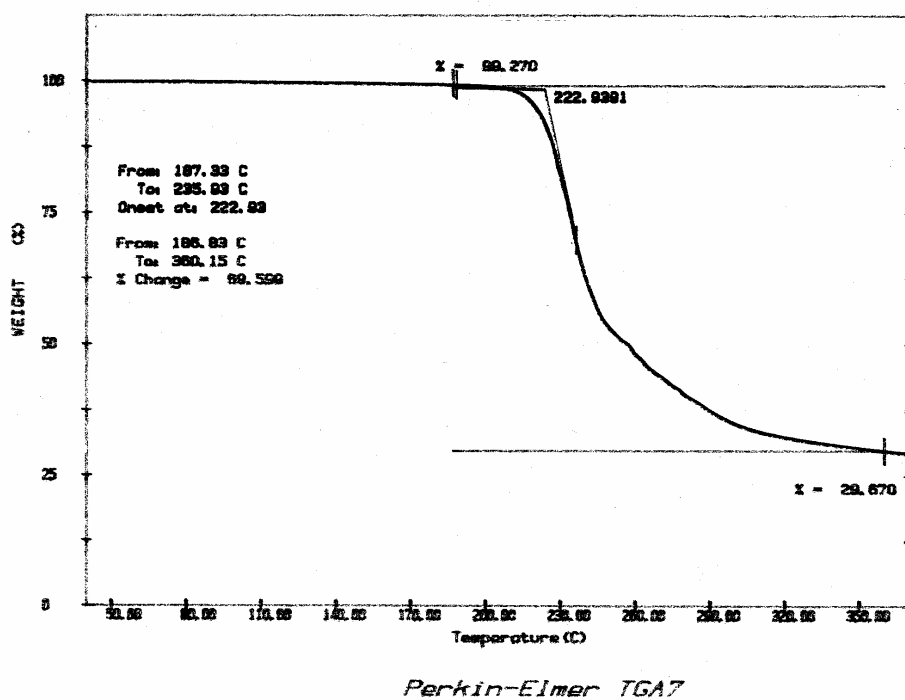Temperature (C)

Perkin-Elmer TGA7

Figure S8. TG analysis of the more-soluble salt

B) For less-soluble salt

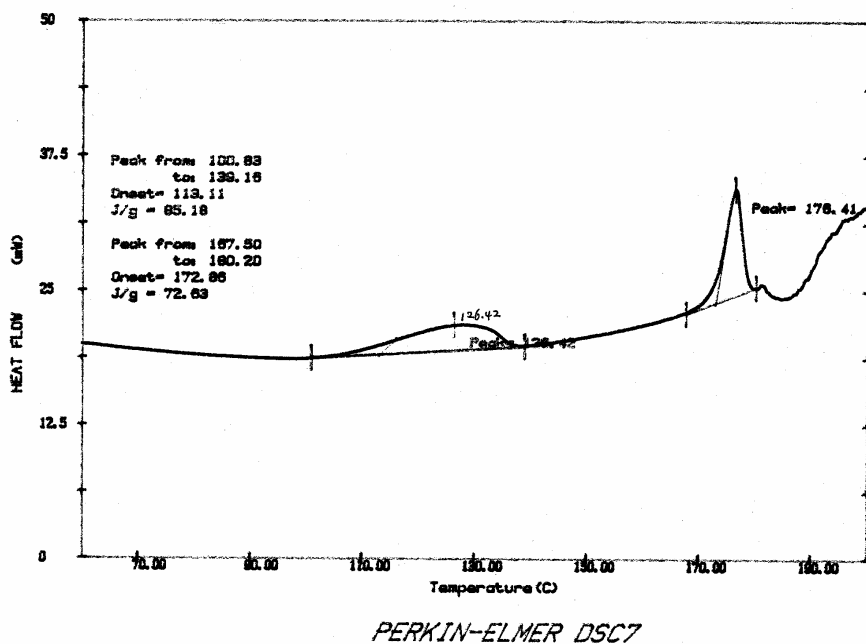**Figure S9.** DSC analysis of the less-soluble salt. $\Delta H_{fus.}$ = (85.18 ×629/1000)+(72.63×611/1000)
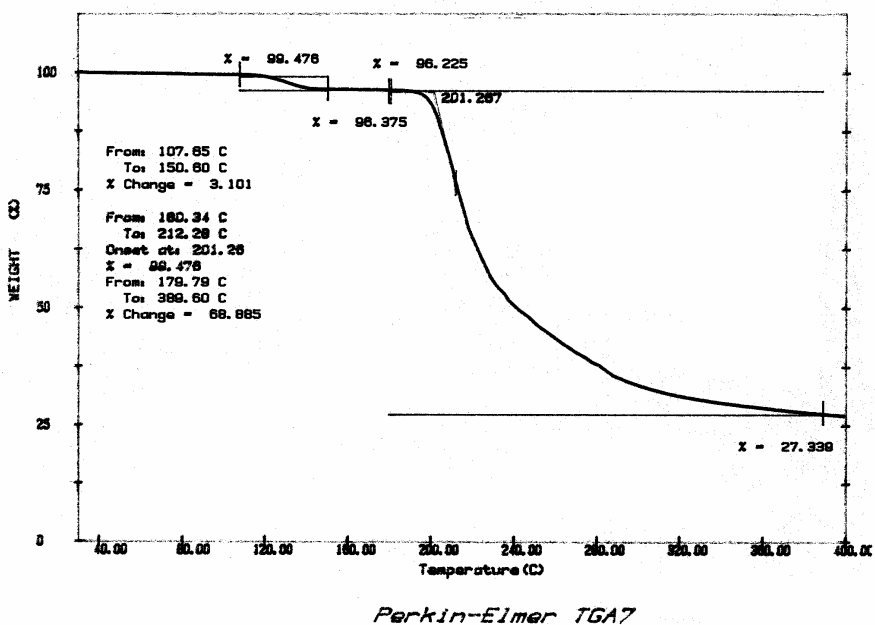= 53.6+44.4 = 98.0 KJ/mol, the first curve is relative to water loss (ΔH = 53.6 KJ/mol)

Figure S10. TG analysis of the less-soluble salt