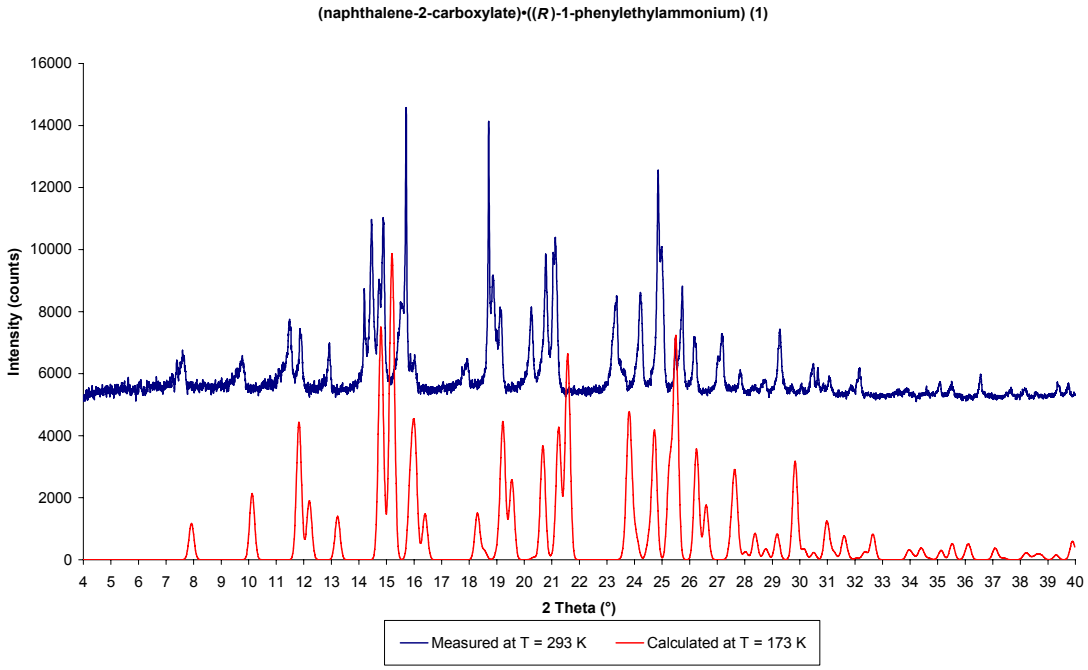
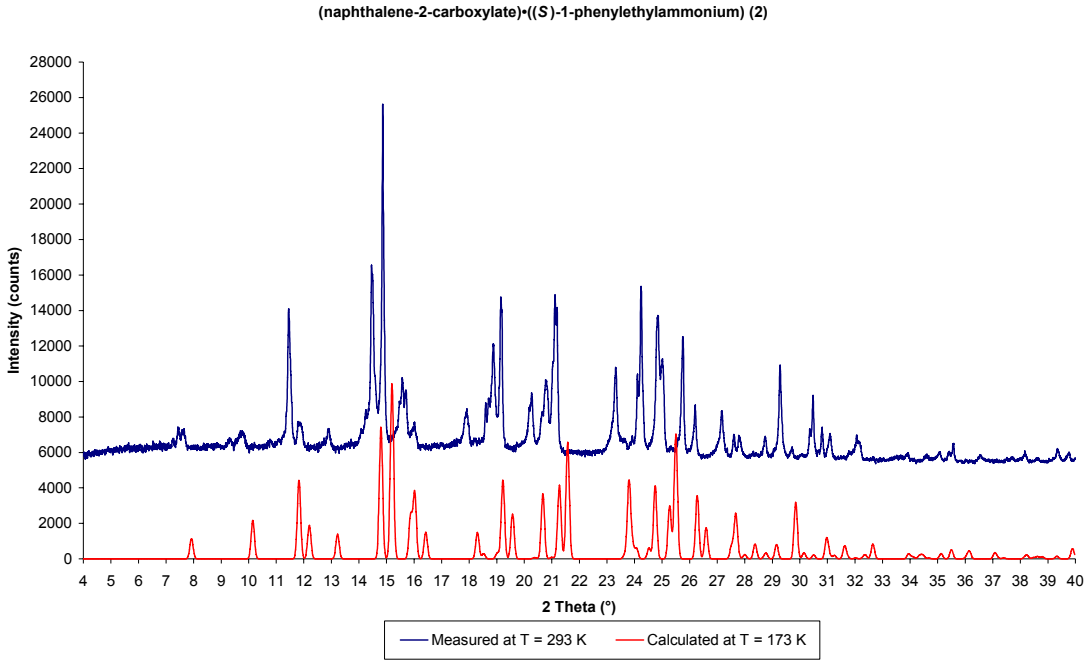
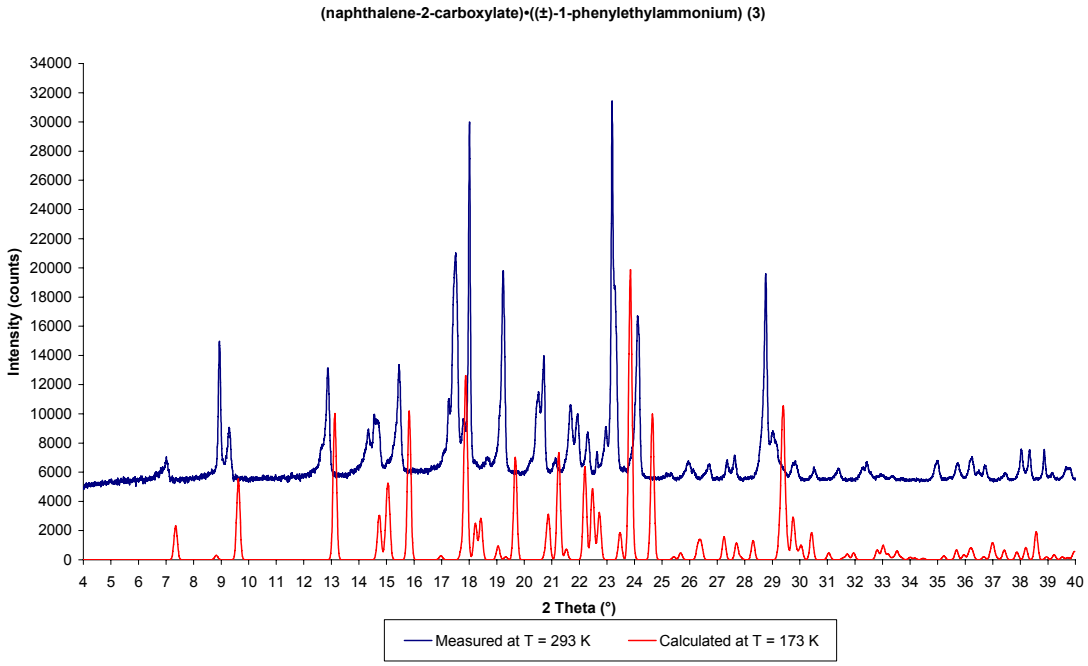
Electronic Supplementary Material for CrystEngComm

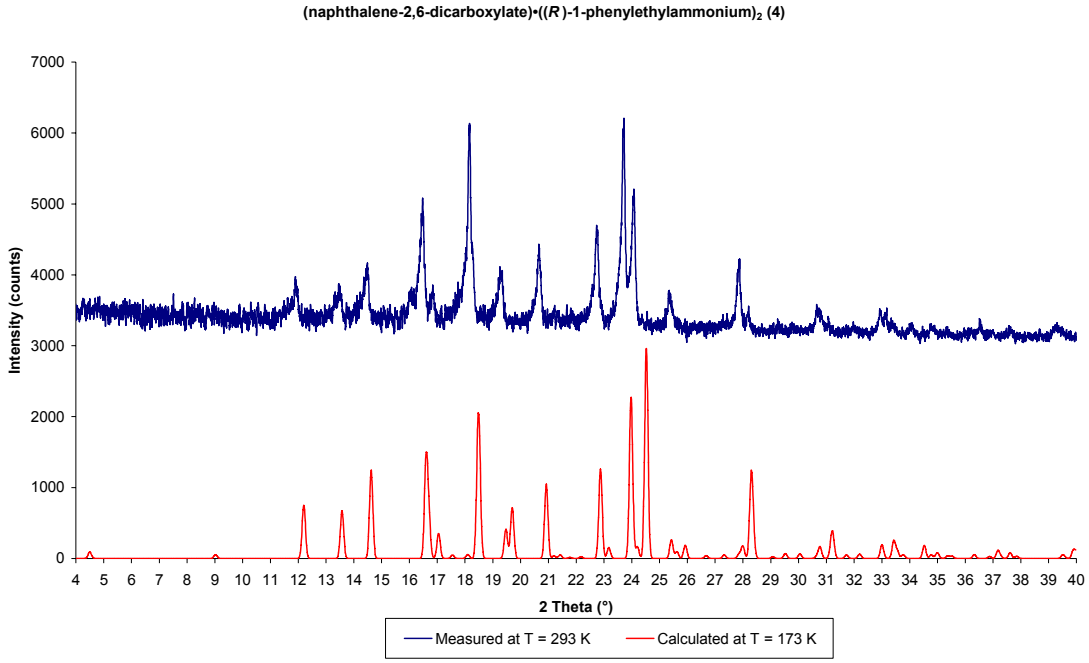
X-ray Powder Diffraction to confirm bulk materials

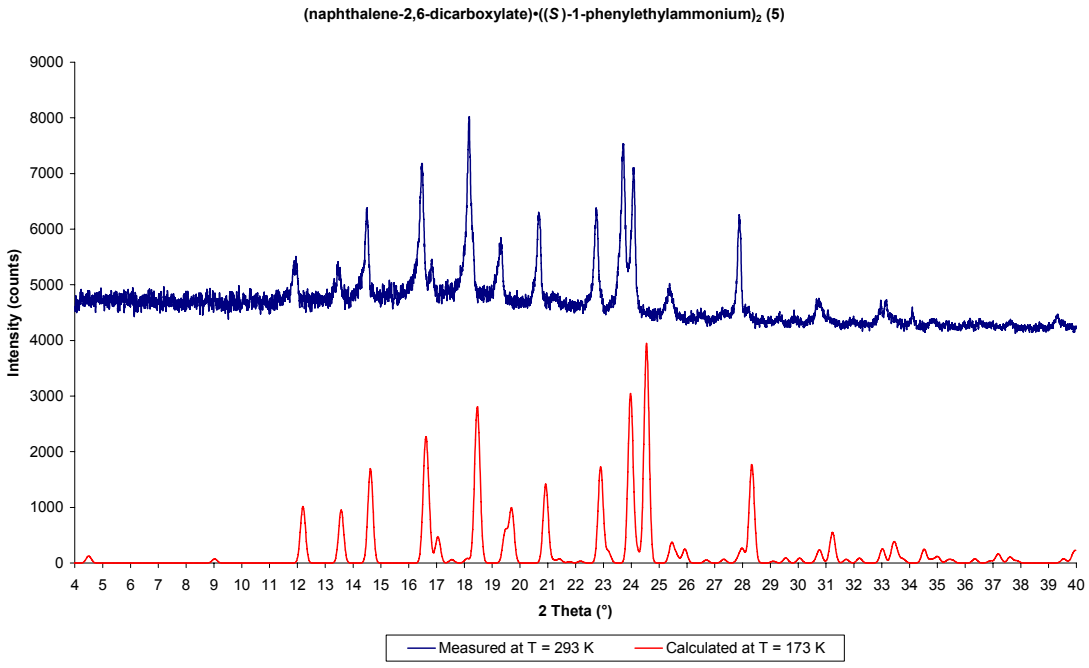
X-ray powder diffraction (HUBER Guinier 670 Imaging Plate diffractometer with Cu K_α radiation, 1.542 A°) at T = 293 K established that the bulk material had the same crystal structure as the crystals selected for single-crystal analysis. The peak positions vary due to the different temperatures at which the measured sample was done compared to the calculated pattern. The peak intensities vary, perhaps due to microcrystalline orientation and/or texture effects.

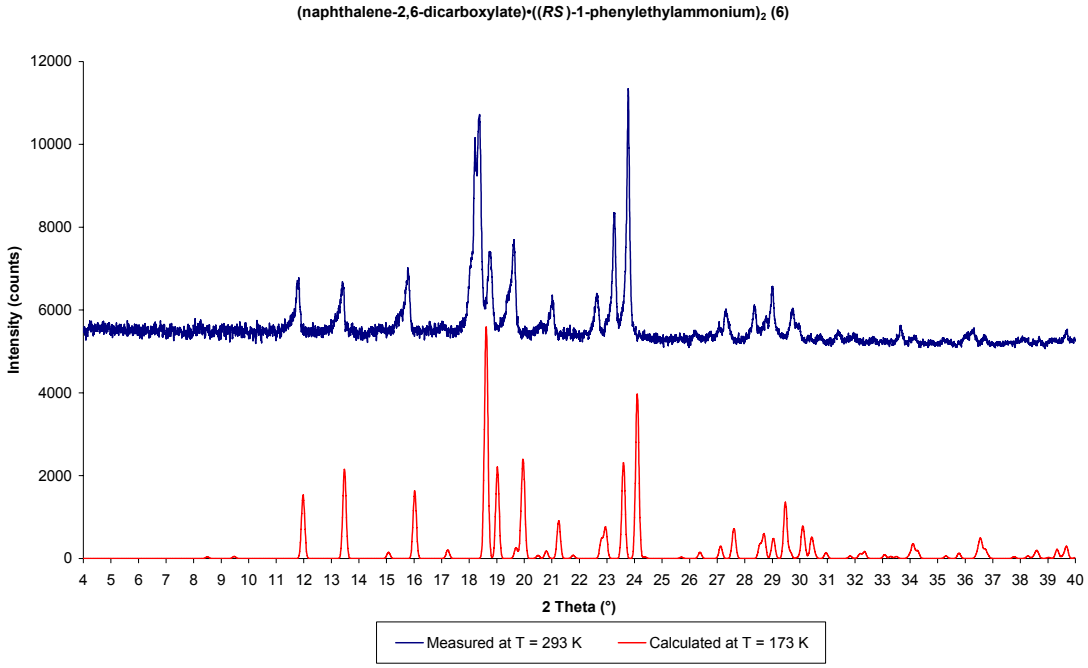



(naphthalene-2-carboxylate)•((S)-1-phenylethylammonium) (2)
Intensity (counts)
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K

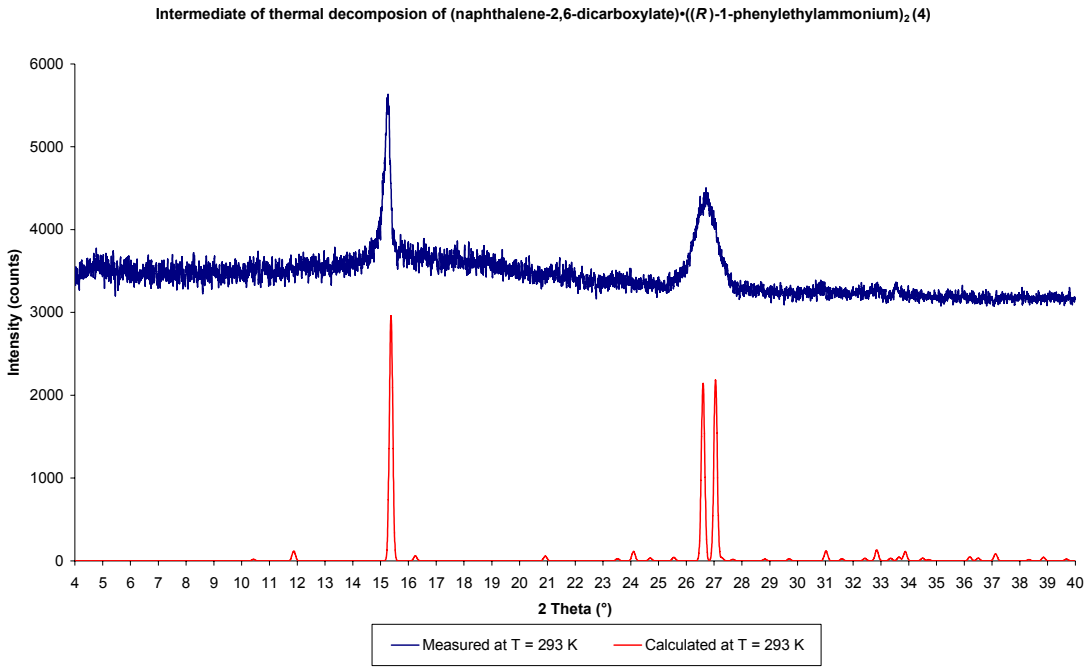

(naphthalene-2-carboxylate)•((±)-1-phenylethylammonium) (3)
Intensity (counts)
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K

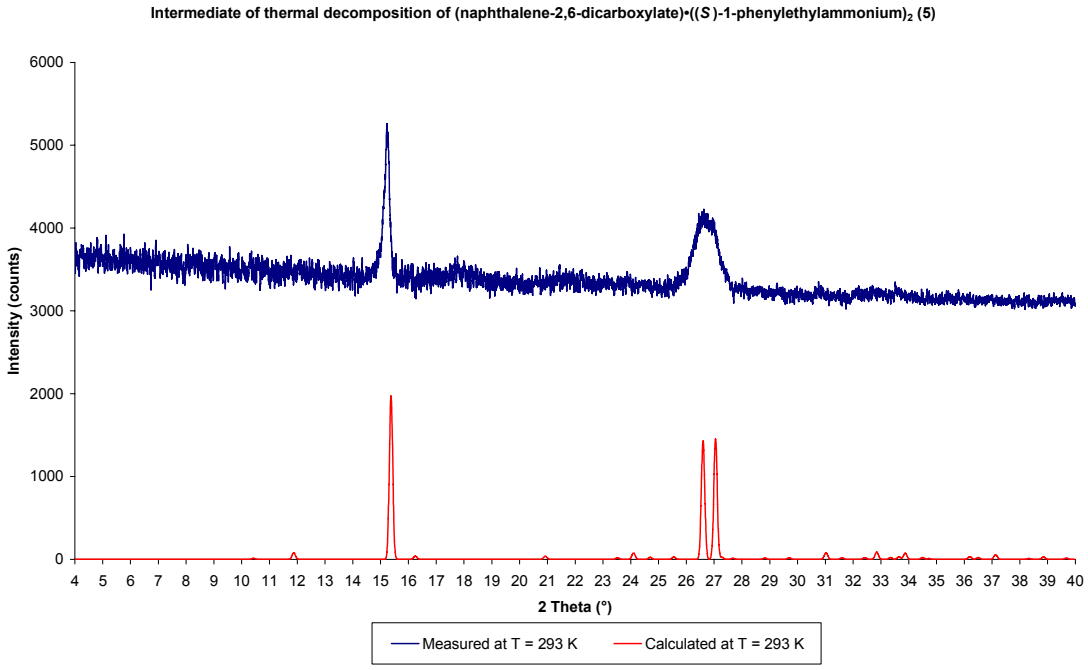

(naphthalene-2,6-dicarboxylate)•((R)-1-phenylethylammonium)2 (4)
Intensity (counts)
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K

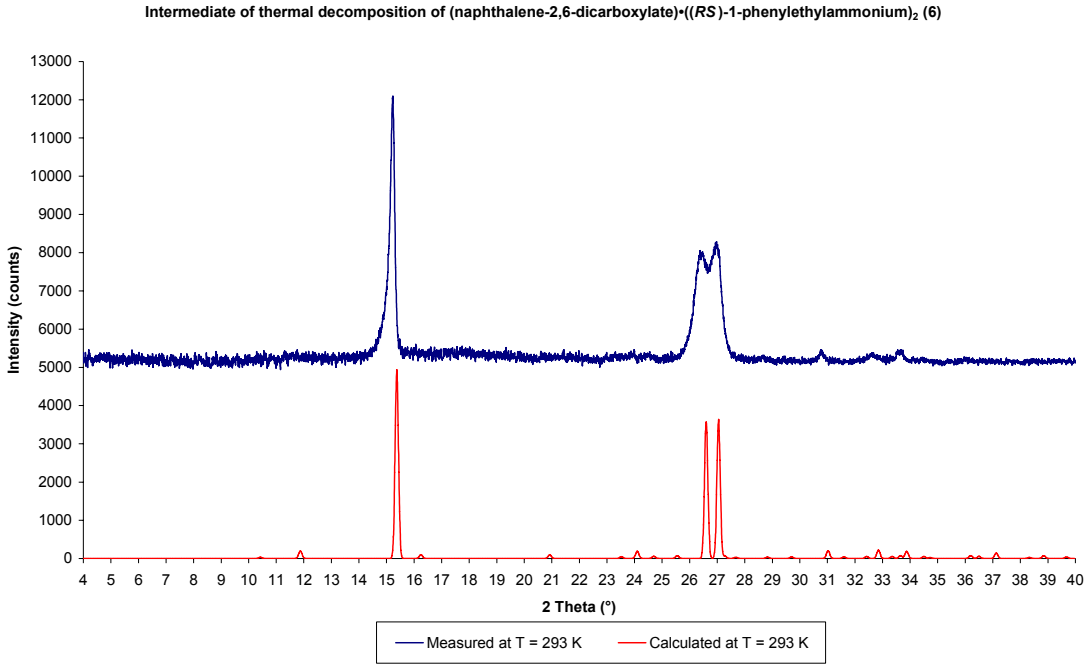

(naphthalene-2,6-dicarboxylate)•((S)-1-phenylethylammonium)2 (5)
Intensity (counts)
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K


(naphthalene-2,6-dicarboxylate)•((RS)-1-phenylethylammonium)2 (6)
Intensity (counts)
12000
10000
8000
6000
4000
2000
0
4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
2 Theta (°)
Measured at T = 293 K
Calculated at T = 173 K

X-ray Powder Diffraction to identify intermediate product formed on thermal decomposition of 4-6.

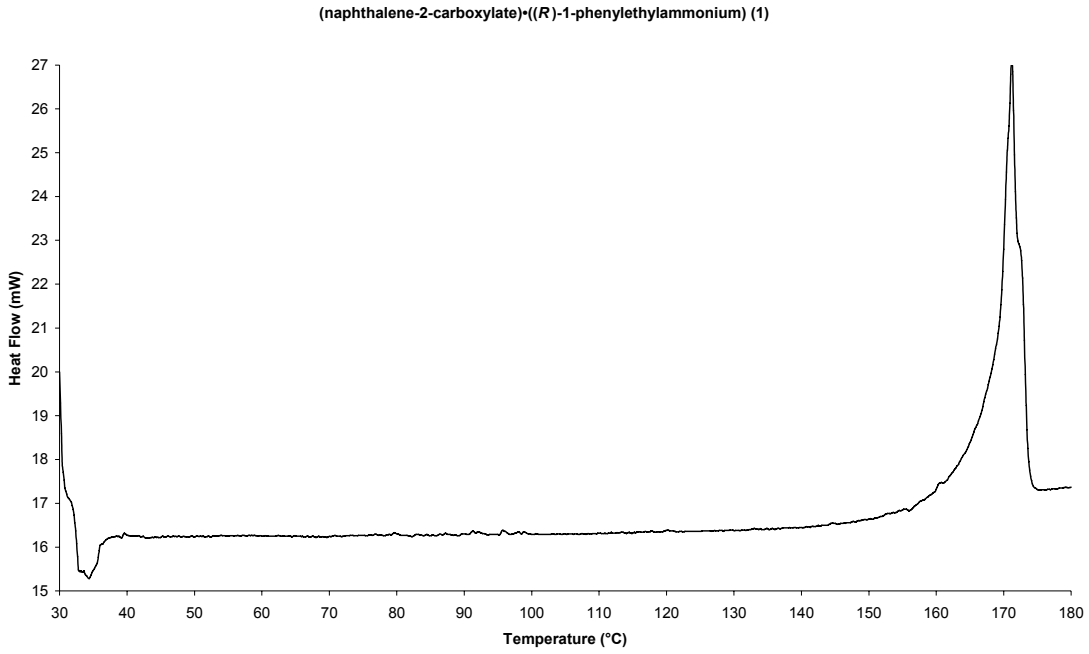


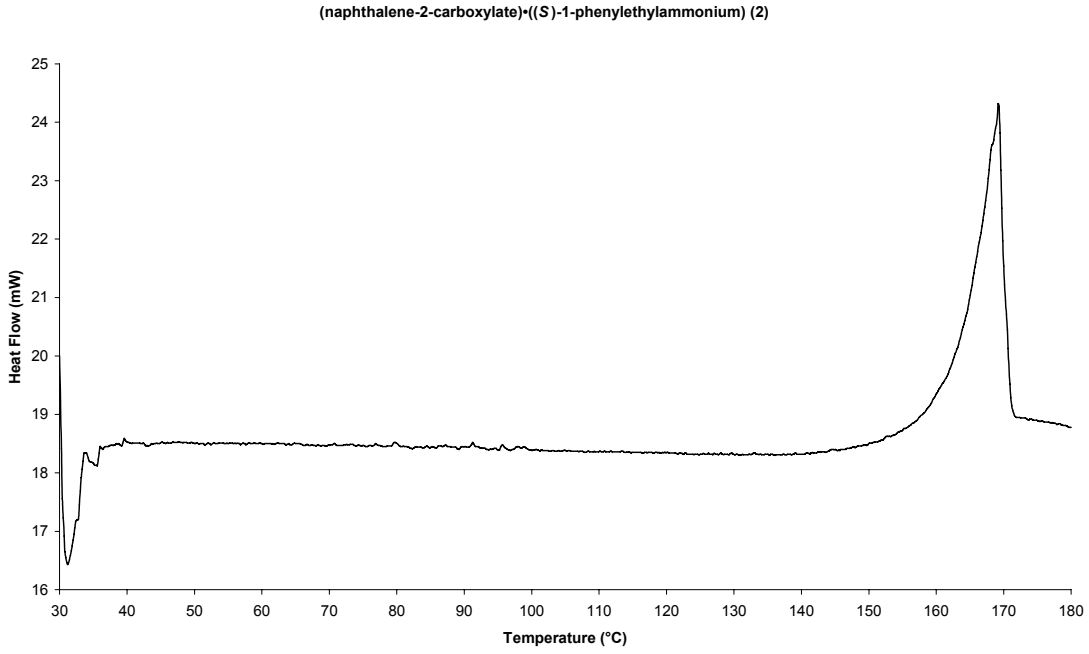


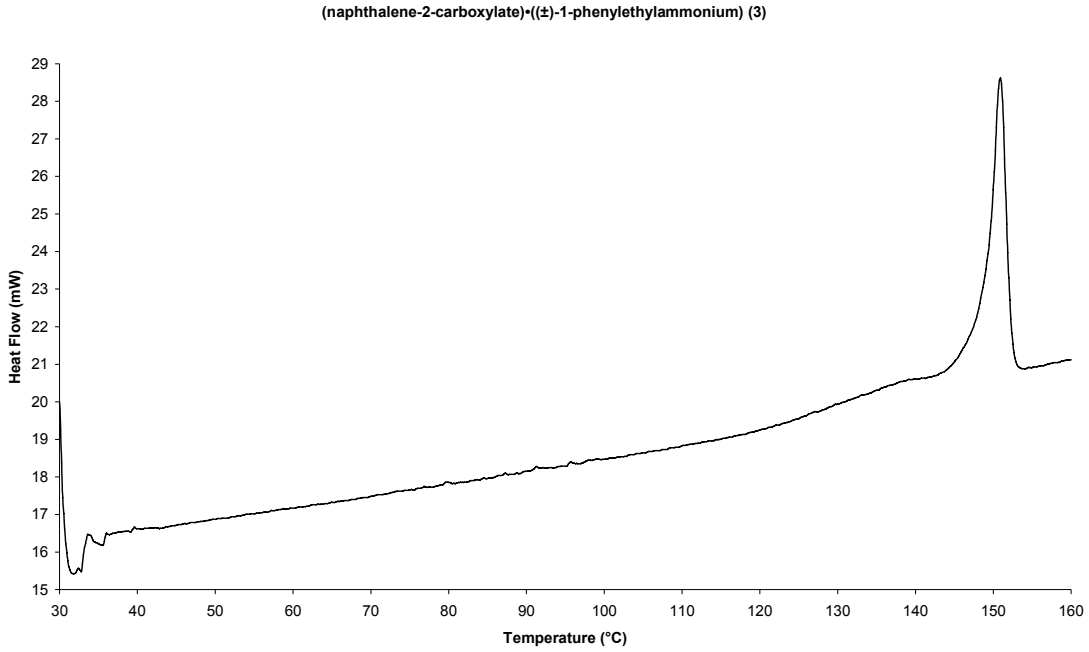

Intermediate of thermal decomposition of (naphthalene-2,6-dicarboxylate)•((RS)-1-phenylethylammonium)2 (6)
Intensity (counts)
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40
2 Theta (°)
Measured at T = 293 K
Calculated at T = 293 K

Differential Scanning Calorimetry

Differential scanning calorimetry was performed using a Perkin Elmer DSC7, heating rate 10°C min^{-1} under an atmosphere of dry N_2 flowing at 4 cm^3 min^{-1}.

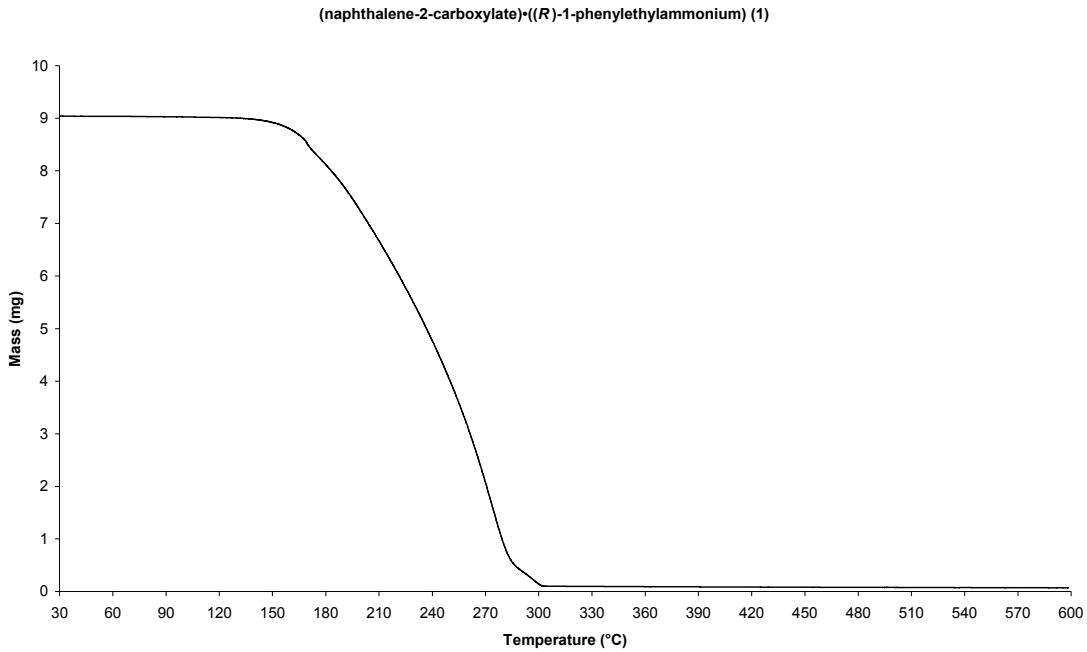


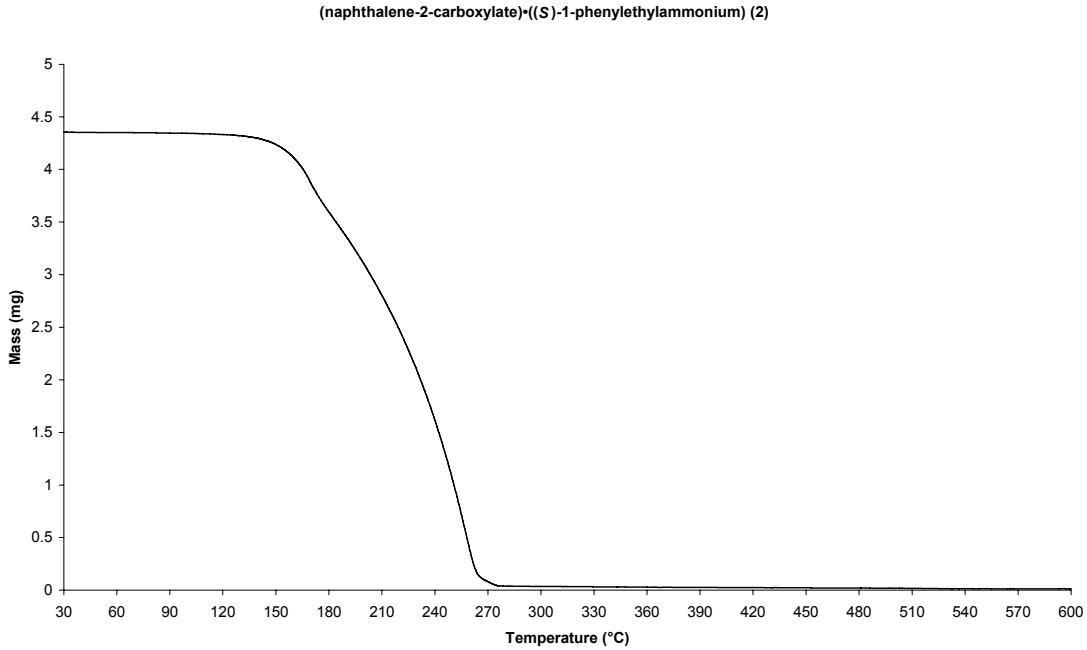


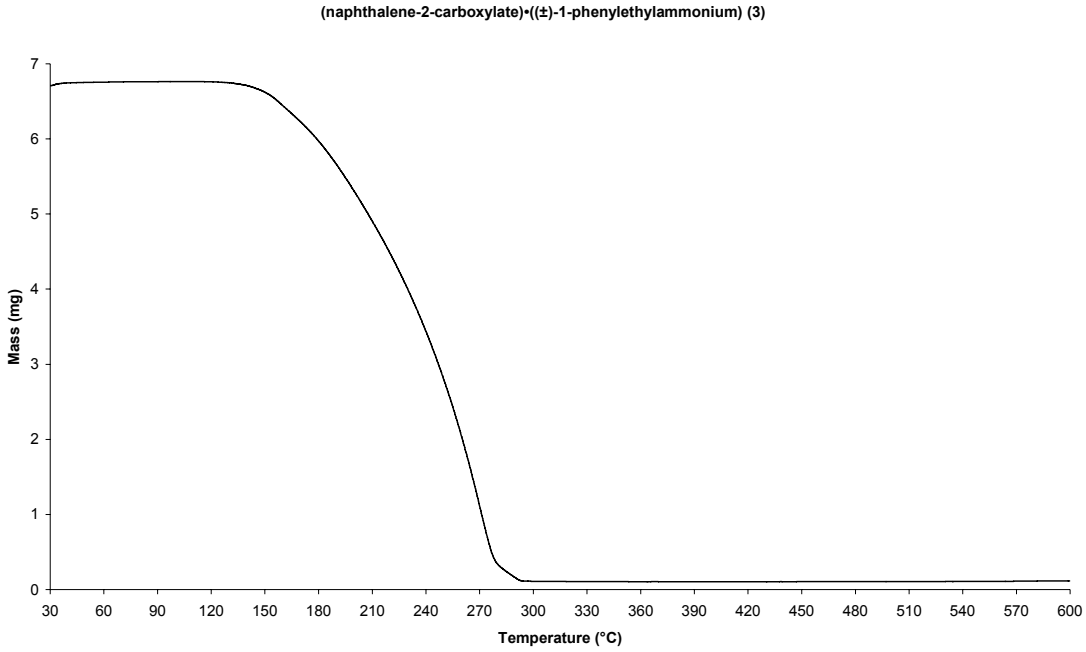

(naphthalene-2-carboxylate)•((±)-1-phenylethylammonium) (3)
Heat Flow (mW)
Temperature (°C)
29
28
27
26
25
24
23
22
21
20
19
18
17
16
15
30
40
50
60
70
80
90
100
110
120
130
140
150
160

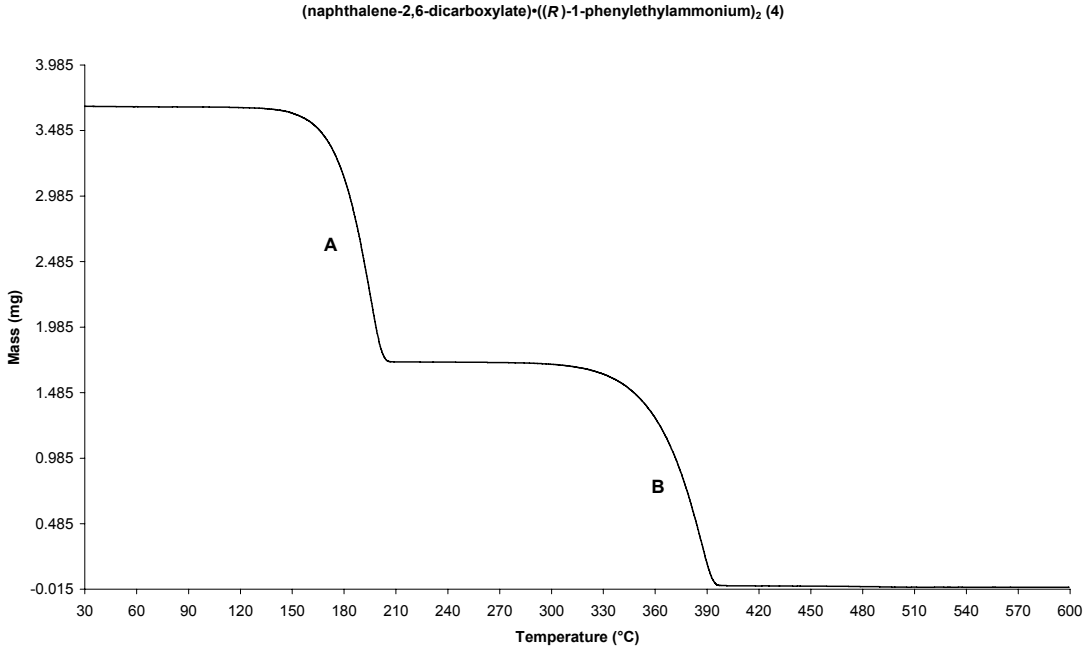
Thermal Gravimetric Analysis

Thermogravimetry was performed using a Mettler Toledo TGA/sDTA 851e, heating rate of 10 °C min^{-1} under an atmosphere of dry N_2 flowing at 30 cm^3 min^{-1}.

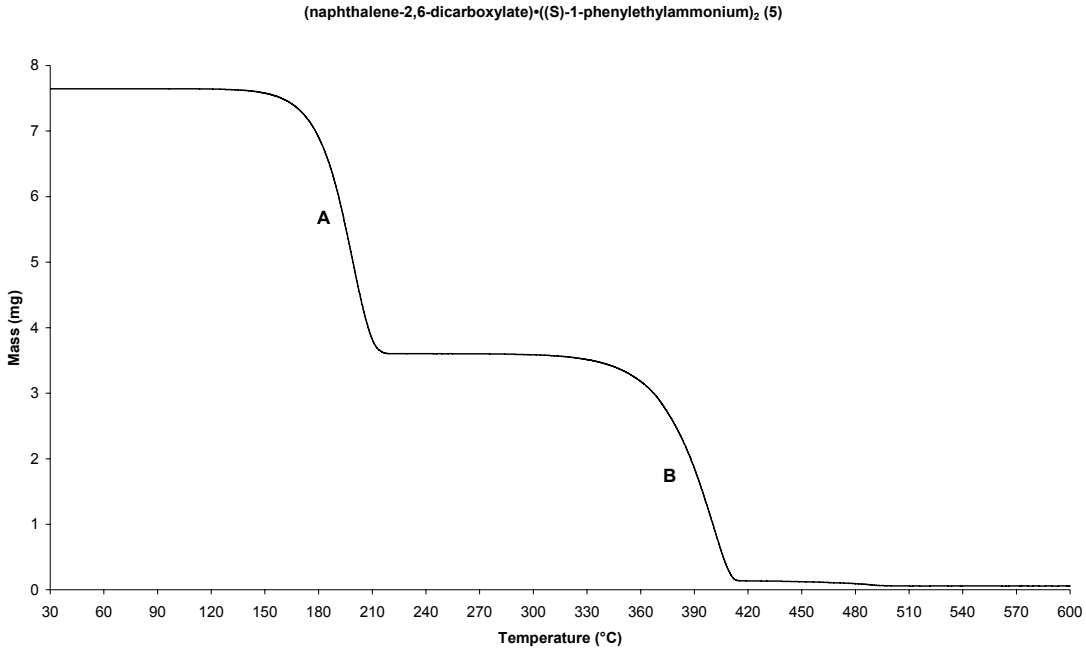




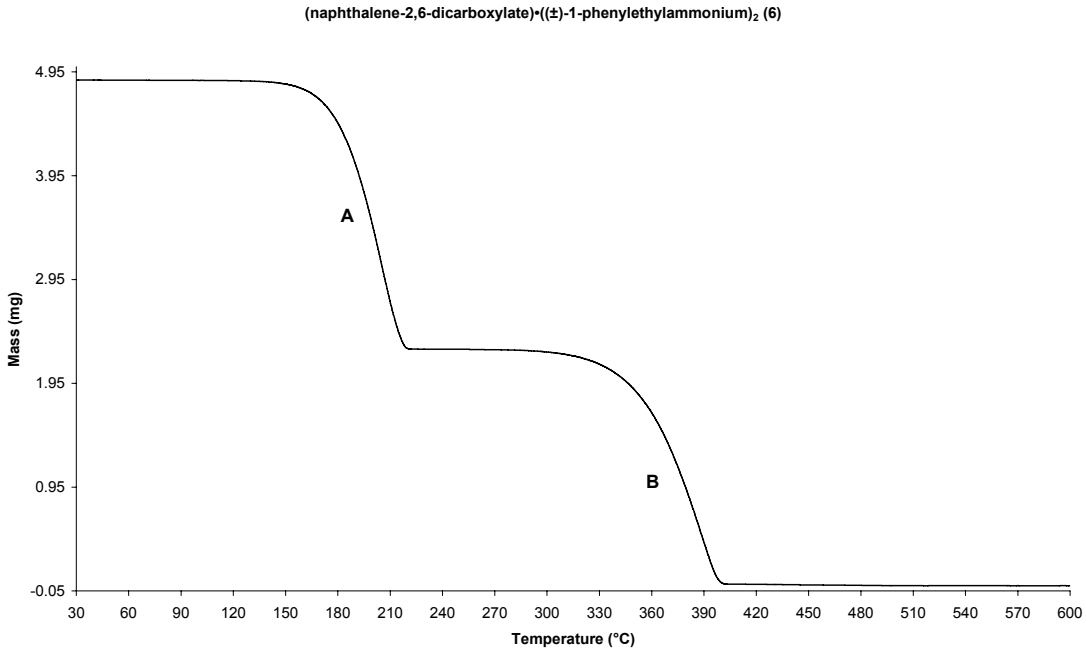




Mass Loss A: 52.87% corresponds to two (R)-1-phenylethylammonium cations
Mass Loss B: 46.41% corresponds to one naphthalene-2,6-dicarboxylate anion



Mass Loss A: 52.90% corresponds to two (S)-1-phenylethylammonium cations
Mass Loss B: 46.34% corresponds to one naphthalene-2,6-dicarboxylate anion



Mass Loss A: 53.05% corresponds to two (*RS*)-1-phenylethylammonium cations
Mass Loss B: 46.49% corresponds to one naphthalene-2,6-dicarboxylate anion