

Figure 1

Ortep plot (50%) with symbol plot for molecule A

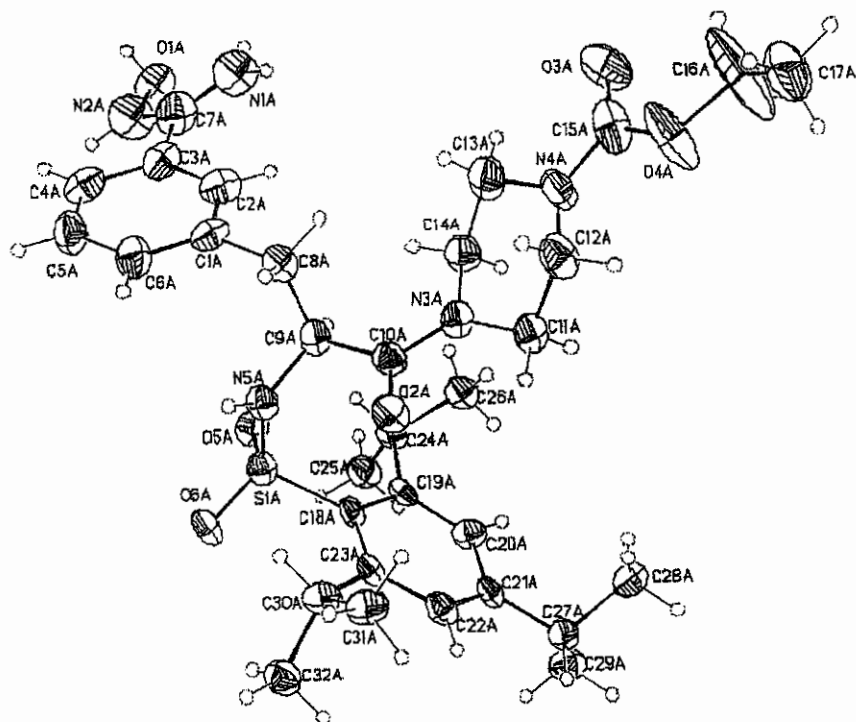


Figure 2

Ortep plot (50%) with symbol plot for molecule B

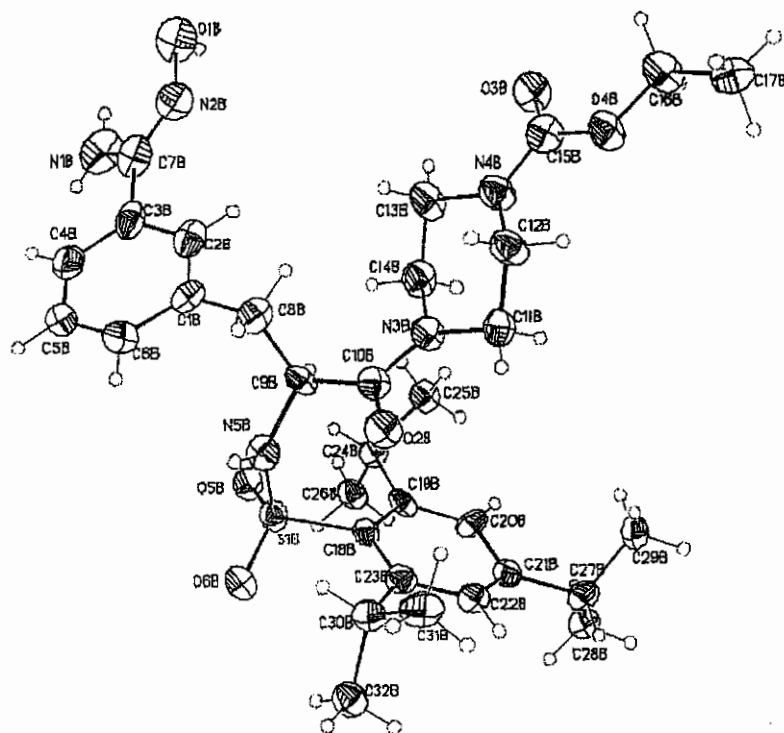


Figure 3

Independent molecules within the unit cell

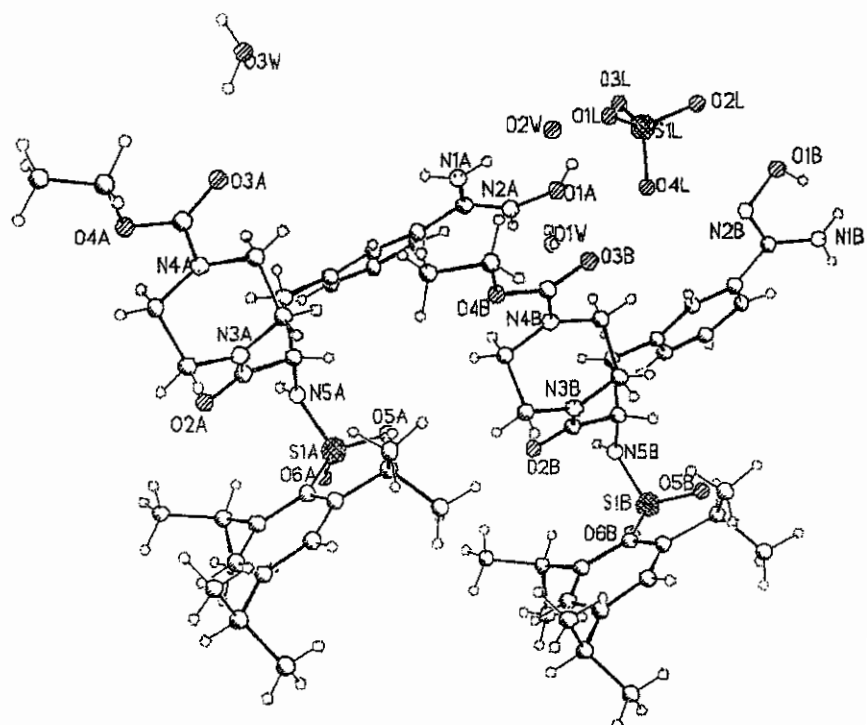


Figure 4

Simulated X-ray diffractogram using the monocrystal data of WX-671.2

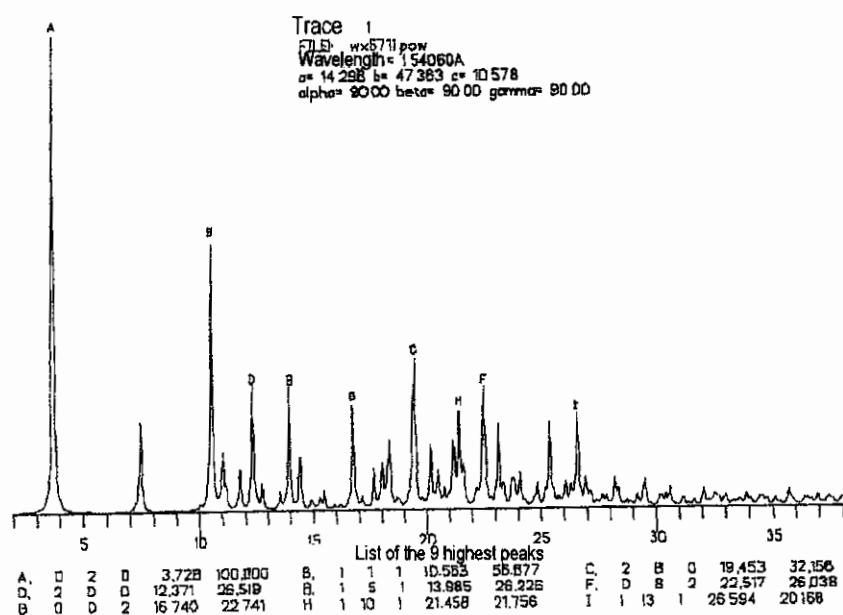


Figure 5

Experimental X-ray diffractogram of WX-671.2

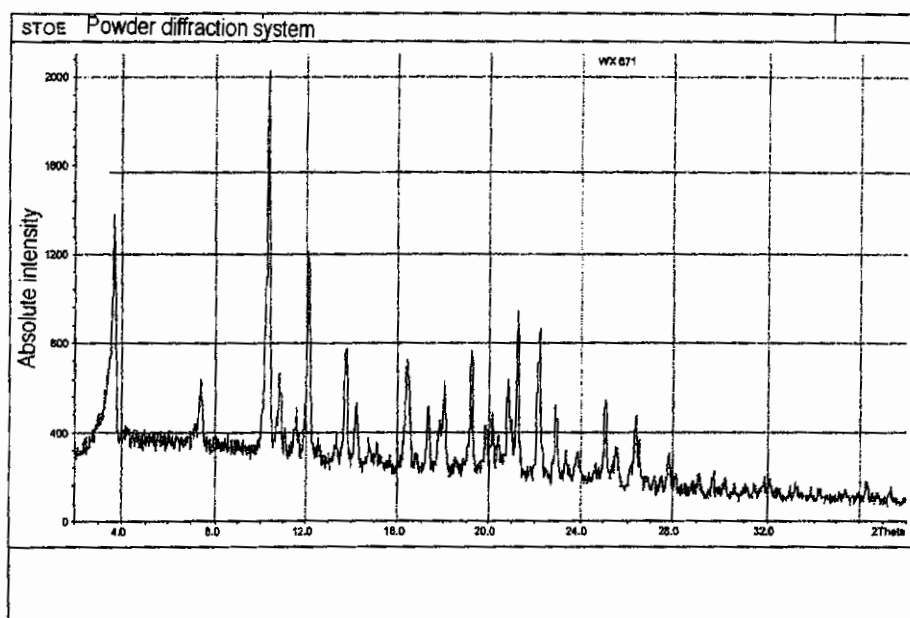
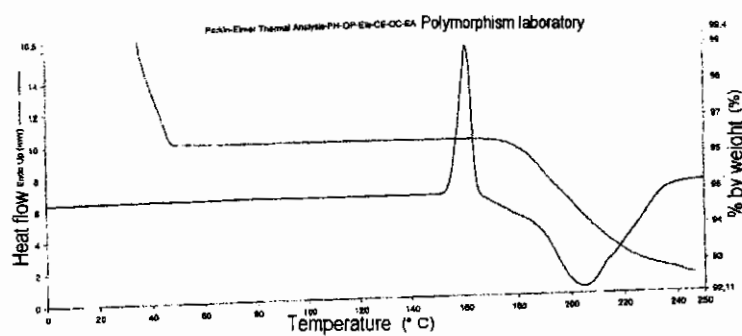
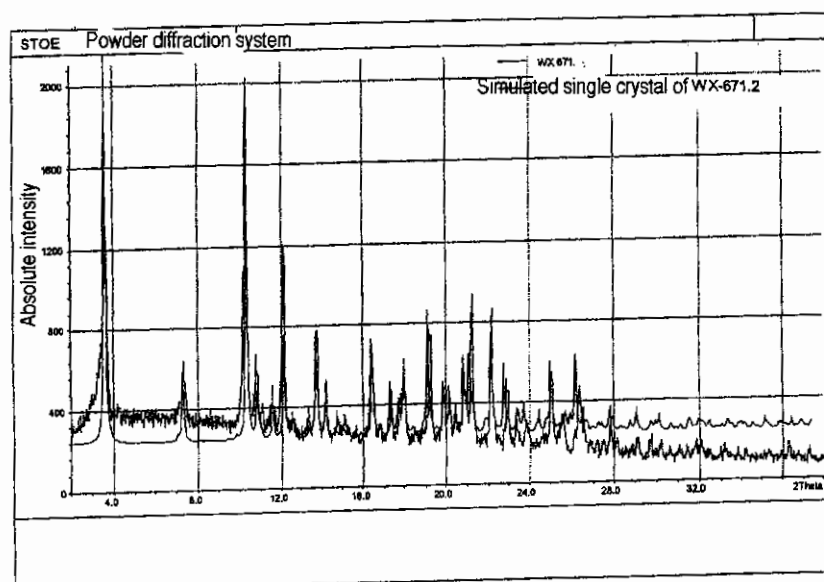


Figure 6a

Superimposition of the simulated X-ray diffractogram and of the experimental X-ray diffractogram of WX-671.2

**Figure 6b**

DSC and TGA thermograms of WX-671.2 after stirring in water

Figure 7

Crystal data and structure refinement for WX-671.2

Empirical formula	C ₆₄ H ₉₈ N ₁₀ O ₁₉ S ₃
Formula weight	1407.70
Temperature	90(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	<i>P</i> 2 ₁ 2 ₁ 2
Unit cell dimensions	<i>a</i> = 14.296(2) Å α = 90°. <i>b</i> = 47.363(8) Å β = 90°. <i>c</i> = 10.5782(17) Å γ = 90°.
Volume	7163(2) Å ³
<i>Z</i>	4
Density (calculated)	1.305 Mg/m ³
Absorption coefficient	1.577 mm ⁻¹
<i>F</i> (000)	3008
Crystal size	0.06 × 0.05 × 0.015 mm ³
Theta range for data collection	1.87 to 71.54°.
Index ranges	-17 ≤ <i>h</i> ≤ 17, -56 ≤ <i>k</i> ≤ 57, -11 ≤ <i>l</i> ≤ 10
Collected reflections	47 840
Independent reflections	12 632 [<i>R</i> (int) = 0.1231]
Completeness at theta = 71.54°	91.1%
Absorption correction	SADABS (Bruker AXS)
Refinement methods	Full-matrix least-squares on <i>F</i> ²
Data/restrictions/parameters	12 632/0/891
Matching test for <i>F</i> ²	1.013
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0801, <i>wR</i> 2 = 0.1705
<i>R</i> indices (all data)	<i>R</i> 1 = 0.1429, <i>wR</i> 2 = 0.2016
Absolute structure parameters	0.03(3)
Extinction coefficient	0.00027(4)
Greatest diff. peak and valley	0.392 and -0.355 e.Å ⁻³

Figure 8

Bond lengths [Å] and angles [°] for WX-671.2

S(1A)-O(5A)	1.424(4)
S(1A)-O(6A)	1.433(4)
S(1A)-N(5A)	1.637(6)
S(1A)-C(18A)	1.783(6)
C(1A)-C(2A)	1.377(10)
C(1A)-C(6A)	1.389(10)
C(1A)-C(8A)	1.490(9)
N(1A)-C(7A)	1.315(10)
N(1A)-O(1A')	1.68(9)
O(1A)-N(2A)	1.394(9)
N(2A)-C(7A)	1.302(10)
C(2A)-C(3A)	1.401(10)
O(2A)-C(10A)	1.224(8)
N(3A)-C(10A)	1.348(8)
N(3A)-C(11A)	1.447(8)
N(3A)-C(14A)	1.476(9)
C(3A)-C(4A)	1.418(10)
C(3A)-C(7A)	1.464(12)
O(3A)-C(15A)	1.238(10)
C(4A)-C(5A)	1.379(11)
N(4A)-C(15A)	1.355(10)
N(4A)-C(13A)	1.455(9)
N(4A)-C(12A)	1.470(9)
O(4A)-C(15A)	1.297(10)
O(4A)-C(16A)	1.487(10)
N(5A)-C(9A)	1.437(8)
C(5A)-C(6A)	1.397(10)
C(8A)-C(9A)	1.551(9)
C(9A)-C(10A)	1.528(9)
C(11A)-C(12A)	1.526(9)
C(13A)-C(14A)	1.496(10)
C(16A)-C(17A)	1.346(12)
C(18A)-C(19A)	1.420(8)
C(18A)-C(23A)	1.428(9)
C(19A)-C(20A)	1.395(9)

Figure 8 (continued)

C(19A)-C(24A)	1.514(9)
C(20A)-C(21A)	1.383(9)
C(21A)-C(22A)	1.369(9)
C(21A)-C(27A)	1.517(9)
C(22A)-C(23A)	1.397(9)
C(23A)-C(30A)	1.510(9)
C(24A)-C(26A)	1.533(9)
C(24A)-C(25A)	1.543(9)
C(27A)-C(28A)	1.531(9)
C(27A)-C(29A)	1.538(9)
C(30A)-C(32A)	1.518(9)
C(30A)-C(31A)	1.522(9)
S(1L)-O(3L)	1.468(6)
S(1L)-O(1L)	1.471(5)
S(1L)-O(2L)	1.479(5)
S(1L)-O(4L)	1.498(5)
N(1B)-C(7B)	1.318(9)
C(1B)-C(2B)	1.382(10)
C(1B)-C(6B)	1.406(10)
C(1B)-C(8B)	1.486(10)
O(1B)-N(2B)	1.389(8)
S(1B)-O(5B)	1.420(5)
S(1B)-O(6B)	1.433(5)
S(1B)-N(5B)	1.651(5)
S(1B)-C(18B)	1.790(6)
N(2B)-C(7B)	1.340(10)
O(2B)-C(10B)	1.226(8)
C(2B)-C(3B)	1.400(10)
N(3B)-C(10B)	1.356(8)
N(3B)-C(14B)	1.455(9)
N(3B)-C(11B)	1.462(8)
O(3B)-C(15B)	1.222(9)
C(3B)-C(4B)	1.379(10)
C(3B)-C(7B)	1.474(11)
O(4B)-C(15B)	1.328(8)
O(4B)-C(16B)	1.470(8)
N(4B)-C(15B)	1.368(9)

Figure 8 (continued)

N(4B)-C(13B)	1.459(8)
N(4B)-C(12B)	1.466(9)
C(4B)-C(5B)	1.408(11)
N(5B)-C(9B)	1.455(8)
C(5B)-C(6B)	1.374(11)
C(8B)-C(9B)	1.555(9)
C(9B)-C(10B)	1.522(9)
C(11B)-C(12B)	1.515(9)
C(13B)-C(14B)	1.516(10)
C(16B)-C(17B)	1.506(10)
C(18B)-C(23B)	1.412(9)
C(18B)-C(19B)	1.419(9)
C(19B)-C(20B)	1.380(9)
C(19B)-C(24B)	1.522(9)
C(20B)-C(21B)	1.394(9)
C(21B)-C(22B)	1.374(9)
C(21B)-C(27B)	1.514(9)
C(22B)-C(23B)	1.390(9)
C(23B)-C(30B)	1.509(9)
C(24B)-C(25B)	1.532(9)
C(24B)-C(26B)	1.538(9)
C(27B)-C(28B)	1.519(9)
C(27B)-C(29B)	1.524(9)
C(30B)-C(31B)	1.527(9)
C(30B)-C(32B)	1.541(9)
O(2W)-O(4W)	1.45(5)
O(5A)-S(1A)-O(6A)	118.8(3)
O(5A)-S(1A)-N(5A)	106.7(3)
O(6A)-S(1A)-N(5A)	105.6(3)
O(5A)-S(1A)-C(18A)	109.5(3)
O(6A)-S(1A)-C(18A)	108.4(3)
N(5A)-S(1A)-C(18A)	107.3(3)
C(2A)-C(1A)-C(6A)	119.0(7)
C(2A)-C(1A)-C(8A)	118.9(7)
C(6A)-C(1A)-C(8A)	122.1(7)
C(7A)-N(1A)-O(1A')	122(3)
C(7A)-N(2A)-O(1A)	116.4(7)

Figure 8 (continued)

C(1A)-C(2A)-C(3A)	122.4(8)
C(10A)-N(3A)-C(11A)	120.8(6)
C(10A)-N(3A)-C(14A)	126.3(6)
C(11A)-N(3A)-C(14A)	112.5(5)
C(2A)-C(3A)-C(4A)	117.9(7)
C(2A)-C(3A)-C(7A)	120.7(7)
C(4A)-C(3A)-C(7A)	121.3(7)
C(5A)-C(4A)-C(3A)	119.6(7)
C(15A)-N(4A)-C(13A)	118.0(7)
C(15A)-N(4A)-C(12A)	122.6(7)
C(13A)-N(4A)-C(12A)	115.9(6)
C(15A)-O(4A)-C(16A)	116.0(8)
C(9A)-N(5A)-S(1A)	121.0(5)
C(4A)-C(5A)-C(6A)	121.0(7)
C(1A)-C(6A)-C(5A)	120.1(7)
N(2A)-C(7A)-N(1A)	121.9(8)
N(2A)-C(7A)-C(3A)	118.9(8)
N(1A)-C(7A)-C(3A)	119.2(8)
C(1A)-C(8A)-C(9A)	112.9(5)
N(5A)-C(9A)-C(10A)	109.9(5)
N(5A)-C(9A)-C(8A)	109.3(5)
C(10A)-C(9A)-C(8A)	108.3(5)
O(2A)-C(10A)-N(3A)	120.3(7)
O(2A)-C(10A)-C(9A)	119.7(6)
N(3A)-C(10A)-C(9A)	120.0(6)
N(3A)-C(11A)-C(12A)	110.5(6)
N(4A)-C(12A)-C(11A)	108.6(6)
N(4A)-C(13A)-C(14A)	110.2(6)
N(3A)-C(14A)-C(13A)	110.2(6)
O(3A)-C(15A)-O(4A)	123.1(8)
O(3A)-C(15A)-N(4A)	123.6(8)
O(4A)-C(15A)-N(4A)	113.3(8)
C(17A)-C(16A)-O(4A)	108.8(8)
C(19A)-C(18A)-C(23A)	119.5(5)
C(19A)-C(18A)-S(1A)	122.1(5)
C(23A)-C(18A)-S(1A)	118.4(5)
C(20A)-C(19A)-C(18A)	117.7(6)

Figure 8 (continued)

C(20A)-C(19A)-C(24A)	116.2(6)
C(18A)-C(19A)-C(24A)	126.1(6)
C(21A)-C(20A)-C(19A)	123.7(6)
C(22A)-C(21A)-C(20A)	117.3(6)
C(22A)-C(21A)-C(27A)	121.5(8)
C(20A)-C(21A)-C(27A)	121.1(6)
C(21A)-C(22A)-C(23A)	123.3(6)
C(22A)-C(23A)-C(18A)	118.2(6)
C(22A)-C(23A)-C(30A)	116.5(6)
C(18A)-C(23A)-C(30A)	125.3(6)
C(19A)-C(24A)-C(26A)	112.9(5)
C(19A)-C(24A)-C(25A)	109.7(5)
C(26A)-C(24A)-C(25A)	109.0(5)
C(21A)-C(27A)-C(28A)	110.2(5)
C(21A)-C(27A)-C(29A)	111.8(5)
C(28A)-C(27A)-C(29A)	109.6(6)
C(23A)-C(30A)-C(32A)	109.1(6)
C(23A)-C(30A)-C(31A)	113.2(5)
C(32A)-C(30A)-C(31A)	109.8(5)
O(3L)-S(1L)-O(1L)	110.3(3)
O(3L)-S(1L)-O(2L)	110.8(3)
O(1L)-S(1L)-O(2L)	108.5(3)
O(3L)-S(1L)-O(4L)	109.7(3)
O(1L)-S(1L)-O(4L)	108.6(3)
O(2L)-S(1L)-O(4L)	108.9(3)
C(2B)-C(1B)-C(6B)	117.0(8)
C(2B)-C(1B)-C(8B)	120.8(7)
C(6B)-C(1B)-C(8B)	122.2(7)
O(5B)-S(1B)-O(6B)	118.1(3)
O(5B)-S(1B)-N(5B)	106.4(3)
O(6B)-S(1B)-N(5B)	105.8(3)
O(5B)-S(1B)-C(18B)	109.9(3)
O(6B)-S(1B)-C(18B)	108.2(3)
N(5B)-S(1B)-C(18B)	107.9(3)
C(7B)-N(2B)-O(1B)	117.8(6)
C(1B)-C(2B)-C(3B)	122.5(7)
C(10B)-N(3B)-C(14B)	125.6(6)

Figure 8 (continued)

C(10B)-N(3B)-C(11B)	120.1(6)
C(14B)-N(3B)-C(11B)	114.0(5)
C(4B)-C(3B)-C(2B)	119.2(8)
C(4B)-C(3B)-C(7B)	121.1(8)
C(2B)-C(3B)-C(7B)	119.6(7)
C(15B)-O(4B)-C(16B)	113.9(5)
C(15B)-N(4B)-C(13B)	119.2(6)
C(15B)-N(4B)-C(12B)	125.1(6)
C(13B)-N(4B)-C(12B)	115.5(6)
C(3B)-C(4B)-C(5B)	119.3(8)
C(9B)-N(5B)-S(1B)	118.2(4)
C(6B)-C(5B)-C(4B)	120.1(7)
C(5B)-C(6B)-C(1B)	121.6(8)
N(1B)-C(7B)-N(2B)	120.9(8)
N(1B)-C(7B)-C(3B)	123.1(8)
N(2B)-C(7B)-C(3B)	116.1(7)
C(1B)-C(8B)-C(9B)	115.3(6)
N(5B)-C(9B)-C(10B)	108.5(5)
N(5B)-C(9B)-C(8B)	108.9(5)
C(10B)-C(9B)-C(8B)	108.1(5)
O(2B)-C(10B)-N(3B)	121.0(7)
O(2B)-C(10B)-C(9B)	119.2(6)
N(3B)-C(10B)-C(9B)	119.6(6)
N(3B)-C(11B)-C(12B)	110.0(5)
N(4B)-C(12B)-C(11B)	109.5(6)
N(4B)-C(13B)-C(14B)	109.8(6)
N(3B)-C(14B)-C(13B)	110.2(6)
O(3B)-C(15B)-O(4B)	125.5(7)
O(3B)-C(15B)-N(4B)	123.2(7)
O(4B)-C(15B)-N(4B)	111.2(6)
O(4B)-C(16B)-C(17B)	105.8(6)
C(23B)-C(18B)-C(19B)	120.4(5)
C(23B)-C(18B)-S(1B)	117.4(5)
C(19B)-C(18B)-S(1B)	122.2(5)
C(20B)-C(19B)-C(18B)	118.0(6)
C(20B)-C(19B)-C(24B)	116.3(6)
C(18B)-C(19B)-C(24B)	125.7(6)

Figure 8 (continued)

C(19B)-C(20B)-C(21B)	123.3(6)
C(22B)-C(21B)-C(20B)	116.4(6)
C(22B)-C(21B)-C(27B)	122.1(6)
C(20B)-C(21B)-C(27B)	121.3(6)
C(21B)-C(22B)-C(23B)	124.4(6)
C(22B)-C(23B)-C(18B)	117.2(6)
C(22B)-C(23B)-C(30B)	115.8(6)
C(18B)-C(23B)-C(30B)	127.0(6)
C(19B)-C(24B)-C(25B)	112.3(5)
C(19B)-C(24B)-C(26B)	109.3(5)
C(25B)-C(24B)-C(26B)	110.8(5)
C(21B)-C(27B)-C(28B)	111.2(6)
C(21B)-C(27B)-C(29B)	111.1(5)
C(28B)-C(27B)-C(29B)	110.6(6)
C(23B)-C(30B)-C(31B)	113.5(5)
C(23B)-C(30B)-C(32B)	109.3(6)
C(31B)-C(30B)-C(32B)	110.4(5)

Figure 9Torsion angles [$^{\circ}$] for WX-671.2

C(6A)-C(1A)-C(2A)-C(3A)	-0.5(11)	C(8A)-C(9A)-C(10A)-N(3A)	-81.2(8)
C(8A)-C(1A)-C(2A)-C(3A)	178.3(6)	C(10A)-N(3A)-C(11A)-C(12A)	-114.5(7)
C(1A)-C(2A)-C(3A)-C(4A)	-1.0(11)	C(14A)-N(3A)-C(11A)-C(12A)	58.6(8)
C(1A)-C(2A)-C(3A)-C(7A)	-179.9(7)	C(15A)-N(4A)-C(12A)-C(11A)	-148.4(7)
C(2A)-C(3A)-C(4A)-C(5A)	1.1(11)	C(13A)-N(4A)-C(12A)-C(11A)	53.3(9)
C(7A)-C(3A)-C(4A)-C(5A)	180.0(7)	N(3A)-C(11A)-C(12A)-N(4A)	-53.8(8)
O(5A)-S(1A)-N(5A)-C(9A)	-57.5(5)	C(15A)-N(4A)-C(13A)-C(14A)	146.9(7)
O(6A)-S(1A)-N(5A)-C(9A)	175.2(5)	C(12A)-N(4A)-C(13A)-C(14A)	-53.8(9)
C(18A)-S(1A)-N(5A)-C(9A)	59.8(5)	C(10A)-N(3A)-C(14A)-C(13A)	114.5(7)
C(3A)-C(4A)-C(5A)-C(6A)	0.4(12)	C(11A)-N(3A)-C(14A)-C(13A)	-58.1(8)
C(2A)-C(1A)-C(6A)-C(5A)	2.0(11)	N(4A)-C(13A)-C(14A)-N(3A)	53.1(8)
C(8A)-C(1A)-C(6A)-C(5A)	-176.8(7)	C(16A)-O(4A)-C(15A)-O(3A)	-8.1(14)
C(4A)-C(5A)-C(6A)-C(1A)	-1.9(11)	C(16A)-O(4A)-C(15A)-N(4A)	170.7(9)
O(1A)-N(2A)-C(7A)-N(1A)	8.5(12)	C(13A)-N(4A)-C(15A)-O(3A)	-13.0(12)
O(1A)-N(2A)-C(7A)-C(3A)	-168.6(7)	C(12A)-N(4A)-C(15A)-O(3A)	-170.9(8)
O(1A)-N(1A)-C(7A)-N(2A)	40(4)	C(13A)-N(4A)-C(15A)-O(4A)	168.2(7)
O(1A)-N(1A)-C(7A)-C(3A)	-143(4)	C(12A)-N(4A)-C(15A)-O(4A)	10.3(11)
C(2A)-C(3A)-C(7A)-N(2A)	152.6(8)	C(15A)-O(4A)-C(16A)-C(17A)	158.6(10)
C(4A)-C(3A)-C(7A)-N(2A)	-26.3(12)	O(5A)-S(1A)-C(18A)-C(19A)	10.6(6)
C(2A)-C(3A)-C(7A)-N(1A)	-24.6(12)	O(6A)-S(1A)-C(18A)-C(19A)	141.6(5)
C(4A)-C(3A)-C(7A)-N(1A)	156.6(8)	N(5A)-S(1A)-C(18A)-C(19A)	-104.8(5)
C(2A)-C(1A)-C(8A)-C(9A)	-85.0(8)	O(5A)-S(1A)-C(18A)-C(23A)	-168.3(4)
C(6A)-C(1A)-C(8A)-C(9A)	93.7(8)	O(6A)-S(1A)-C(18A)-C(23A)	-37.2(5)
S(1A)-N(5A)-C(9A)-C(10A)	-90.1(6)	N(5A)-S(1A)-C(18A)-C(23A)	76.3(5)
S(1A)-N(5A)-C(9A)-C(8A)	151.2(5)	C(23A)-C(18A)-C(19A)-C(20A)	4.2(8)
C(1A)-C(8A)-C(9A)-N(5A)	-64.4(7)	S(1A)-C(18A)-C(19A)-C(20A)	-174.7(4)
C(1A)-C(8A)-C(9A)-C(10A)	175.9(6)	C(23A)-C(18A)-C(19A)-C(24A)	-177.5(5)
C(11A)-N(3A)-C(10A)-O(2A)	-4.4(10)	S(1A)-C(18A)-C(19A)-C(24A)	3.7(8)
C(14A)-N(3A)-C(10A)-O(2A)	-176.5(6)	C(18A)-C(19A)-C(20A)-C(21A)	-1.0(9)
C(11A)-N(3A)-C(10A)-C(9A)	174.3(6)	C(24A)-C(19A)-C(20A)-C(21A)	-179.5(6)
C(14A)-N(3A)-C(10A)-C(9A)	2.2(10)	C(19A)-C(20A)-C(21A)-C(22A)	-2.6(10)
N(5A)-C(9A)-C(10A)-O(2A)	-21.9(9)	C(19A)-C(20A)-C(21A)-C(27A)	-179.6(6)
C(8A)-C(9A)-C(10A)-O(2A)	97.4(7)	C(20A)-C(21A)-C(22A)-C(23A)	3.1(9)
N(5A)-C(9A)-C(10A)-N(3A)	159.5(6)	C(27A)-C(21A)-C(22A)-C(23A)	-179.9(6)

Figure 9 (continued)

C(21A)-C(22A)-C(23A)-C(18A)	0.0(9)	C(2B)-C(1B)-C(8B)-C(9B)	-98.9(8)
C(21A)-C(22A)-C(23A)-C(30A)	179.4(6)	C(6B)-C(1B)-C(8B)-C(9B)	82.0(9)
C(19A)-C(18A)-C(23A)-C(22A)	-3.7(8)	S(1B)-N(5B)-C(9B)-C(10B)	-93.8(6)
S(1A)-C(18A)-C(23A)-C(22A)	175.2(4)	S(1B)-N(5B)-C(9B)-C(8B)	148.8(5)
C(19A)-C(18A)-C(23A)-C(30A)	176.9(6)	C(1B)-C(8B)-C(9B)-N(5B)	-73.8(8)
S(1A)-C(18A)-C(23A)-C(30A)	-4.2(8)	C(1B)-C(8B)-C(9B)-C(10B)	168.5(6)
C(20A)-C(19A)-C(24A)-C(26A)	-39.9(8)	C(14B)-N(3B)-C(10B)-O(2B)	-176.7(7)
C(18A)-C(19A)-C(24A)-C(26A)	141.7(6)	C(11B)-N(3B)-C(10B)-O(2B)	-3.6(10)
C(20A)-C(19A)-C(24A)-C(25A)	81.9(7)	C(14B)-N(3B)-C(10B)-C(9B)	-1.1(10)
C(18A)-C(19A)-C(24A)-C(25A)	-96.5(7)	C(11B)-N(3B)-C(10B)-C(9B)	172.0(6)
C(22A)-C(21A)-C(27A)-C(28A)	-110.2(7)	N(5B)-C(9B)-C(10B)-O(2B)	-22.9(9)
C(20A)-C(21A)-C(27A)-C(28A)	66.7(8)	C(8B)-C(9B)-C(10B)-O(2B)	95.0(7)
C(22A)-C(21A)-C(27A)-C(29A)	127.6(6)	N(5B)-C(9B)-C(10B)-N(3B)	161.5(6)
C(20A)-C(21A)-C(27A)-C(29A)	-55.5(8)	C(8B)-C(9B)-C(10B)-N(3B)	-80.7(8)
C(22A)-C(23A)-C(30A)-C(32A)	-76.7(7)	C(10B)-N(3B)-C(11B)-C(12B)	-116.8(7)
C(18A)-C(23A)-C(30A)-C(32A)	102.7(7)	C(14B)-N(3B)-C(11B)-C(12B)	57.1(8)
C(22A)-C(23A)-C(30A)-C(31A)	45.8(8)	C(15B)-N(4B)-C(12B)-C(11B)	-130.5(7)
C(18A)-C(23A)-C(30A)-C(31A)	-134.8(6)	C(13B)-N(4B)-C(12B)-C(11B)	54.3(9)
C(6B)-C(1B)-C(2B)-C(3B)	-0.6(11)	N(3B)-C(11B)-C(12B)-N(4B)	-53.0(8)
C(8B)-C(1B)-C(2B)-C(3B)	-179.7(6)	C(15B)-N(4B)-C(13B)-C(14B)	130.5(7)
C(1B)-C(2B)-C(3B)-C(4B)	-4.0(11)	C(12B)-N(4B)-C(13B)-C(14B)	-54.1(9)
C(1B)-C(2B)-C(3B)-C(7B)	172.9(7)	C(10B)-N(3B)-C(14B)-C(13B)	116.7(7)
C(2B)-C(3B)-C(4B)-C(5B)	6.4(11)	C(11B)-N(3B)-C(14B)-C(13B)	-56.8(8)
C(7B)-C(3B)-C(4B)-C(5B)	-170.4(7)	N(4B)-C(13B)-C(14B)-N(3B)	52.7(8)
O(5B)-S(1B)-N(5B)-C(9B)	-61.4(5)	C(16B)-O(4B)-C(15B)-O(3B)	-3.4(10)
O(6B)-S(1B)-N(5B)-C(9B)	172.1(5)	C(16B)-O(4B)-C(15B)-N(4B)	175.3(6)
C(18B)-S(1B)-N(5B)-C(9B)	56.5(5)	C(13B)-N(4B)-C(15B)-O(3B)	-5.3(11)
C(3B)-C(4B)-C(5B)-C(6B)	-4.4(12)	C(12B)-N(4B)-C(15B)-O(3B)	179.8(7)
C(4B)-C(5B)-C(6B)-C(1B)	-0.3(13)	C(13B)-N(4B)-C(15B)-O(4B)	176.0(6)
C(2B)-C(1B)-C(6B)-C(5B)	2.7(12)	C(12B)-N(4B)-C(15B)-O(4B)	1.0(10)
C(8B)-C(1B)-C(6B)-C(5B)	-178.2(7)	C(15B)-O(4B)-C(16B)-C(17B)	179.8(6)
O(1B)-N(2B)-C(7B)-N(1B)	1.3(10)	O(5B)-S(1B)-C(18B)-C(23B)	-166.8(4)
O(1B)-N(2B)-C(7B)-C(3B)	-177.9(6)	O(6B)-S(1B)-C(18B)-C(23B)	-36.5(5)
C(4B)-C(3B)-C(7B)-N(1B)	-32.0(11)	N(5B)-S(1B)-C(18B)-C(23B)	77.6(5)
C(2B)-C(3B)-C(7B)-N(1B)	151.2(7)	O(5B)-S(1B)-C(18B)-C(19B)	11.2(6)
C(4B)-C(3B)-C(7B)-N(2B)	147.2(7)	O(6B)-S(1B)-C(18B)-C(19B)	141.5(5)
C(2B)-C(3B)-C(7B)-N(2B)	-29.6(10)	N(5B)-S(1B)-C(18B)-C(19B)	-104.4(5)
		C(23B)-C(18B)-C(19B)-C(20B)	3.6(9)

Figure 9 (continued)

S(1B)-C(18B)-C(19B)-C(20B) -174.4(5)
 C(23B)-C(18B)-C(19B)-C(24B) -176.8(6)
 S(1B)-C(18B)-C(19B)-C(24B) 5.3(8)
 C(18B)-C(19B)-C(20B)-C(21B) 1.9(10)
 C(24B)-C(19B)-C(20B)-C(21B) -177.8(6)
 C(19B)-C(20B)-C(21B)-C(22B) -6.1(10)
 C(19B)-C(20B)-C(21B)-C(27B) 178.3(6)
 C(20B)-C(21B)-C(22B)-C(23B) 5.2(10)
 C(27B)-C(21B)-C(22B)-C(23B) -179.2(6)
 C(21B)-C(22B)-C(23B)-C(18B) -0.1(10)
 C(21B)-C(22B)-C(23B)-C(30B) 179.5(6)
 C(19B)-C(18B)-C(23B)-C(22B) -4.4(9)
 S(1B)-C(18B)-C(23B)-C(22B) 173.6(5)
 C(19B)-C(18B)-C(23B)-C(30B) 176.0(6)
 S(1B)-C(18B)-C(23B)-C(30B) -5.9(8)
 C(20B)-C(19B)-C(24B)-C(25B) -41.4(8)
 C(18B)-C(19B)-C(24B)-C(25B) 138.9(6)
 C(20B)-C(19B)-C(24B)-C(26B) 82.0(7)
 C(18B)-C(19B)-C(24B)-C(26B) -97.7(7)
 C(22B)-C(21B)-C(27B)-C(28B) 127.4(7)
 C(20B)-C(21B)-C(27B)-C(28B) -57.2(8)
 C(22B)-C(21B)-C(27B)-C(29B) -109.0(7)
 C(20B)-C(21B)-C(27B)-C(29B) 66.3(8)
 C(22B)-C(23B)-C(30B)-C(31B) 47.3(8)
 C(18B)-C(23B)-C(30B)-C(31B) -133.2(6)
 C(22B)-C(23B)-C(30B)-C(32B) -76.4(7)
 C(18B)-C(23B)-C(30B)-C(32B) 103.1(7)

Figure 10

DSC and TGA thermograms of WX-671.1 stirred in isopropanol (modification A)

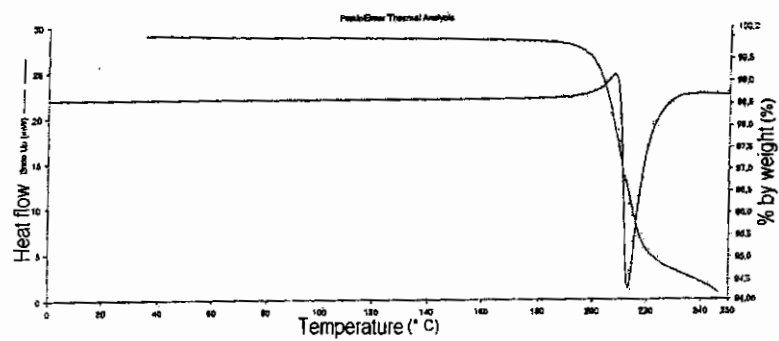


Figure 11

DSC and TGA thermograms of WX-671.1 (mesophase B)

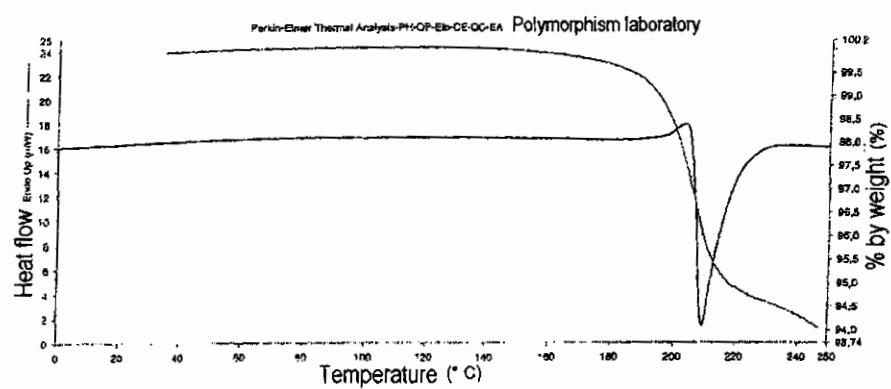


Figure 12

DSC and TGA thermograms of WX-671.1 after crystallization from methanol at room temperature (mesophase C)

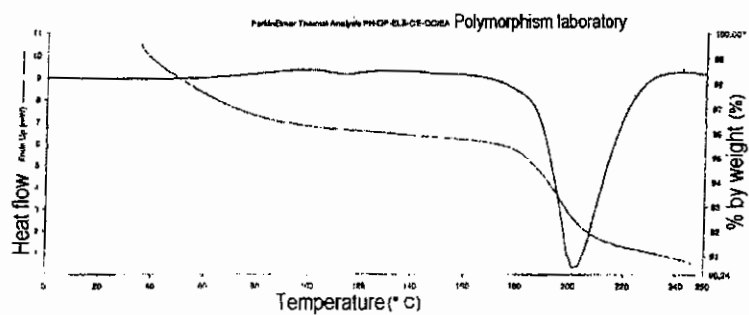


Figure 13

X-ray diffractogram of WX-671.1 after stirring in isopropanol (modification A)

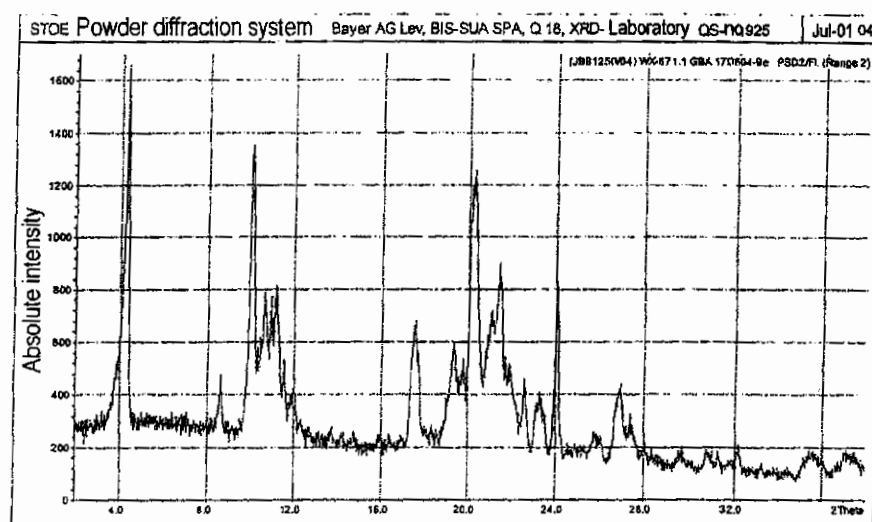


Figure 14

X-ray diffractogram of WX-671.1 (mesophase B)

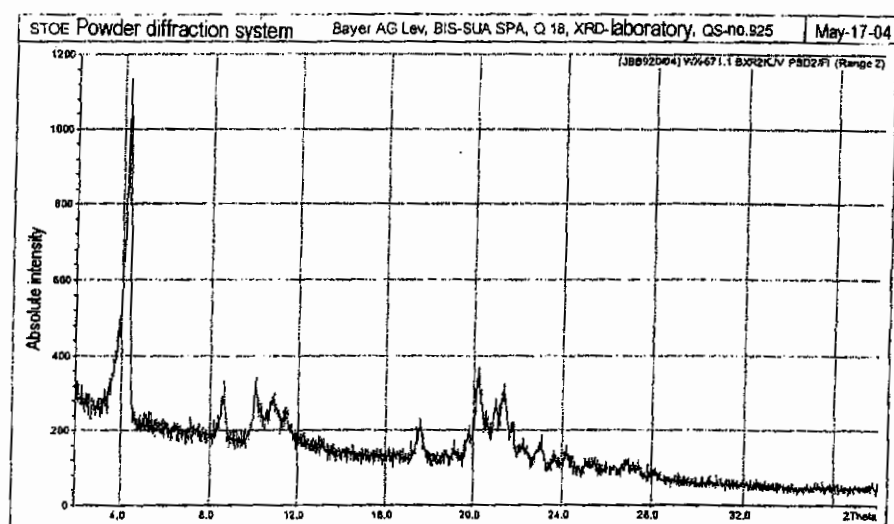


Figure 15

X-ray diffractogram of WX-671.1 after crystallization from methanol at room temperature (mesophase C)

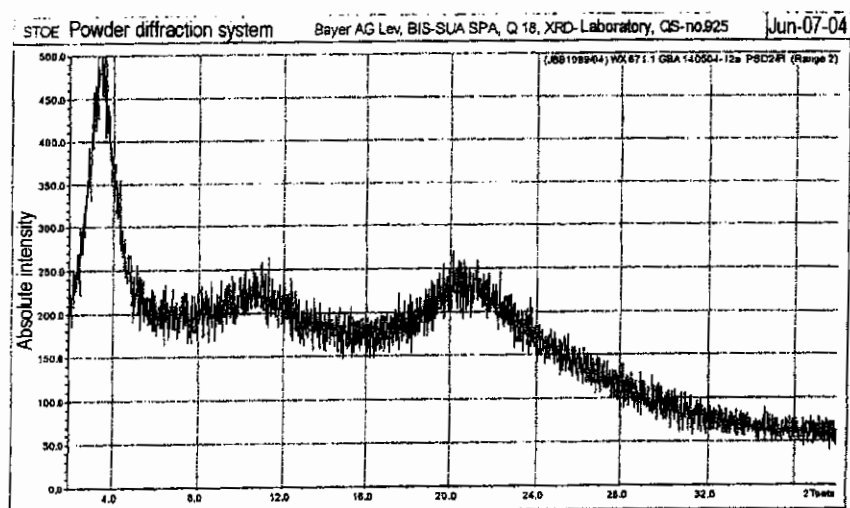


Figure 16

DSC and TGA thermograms of the amorphous starting substance WX-671 (free base)

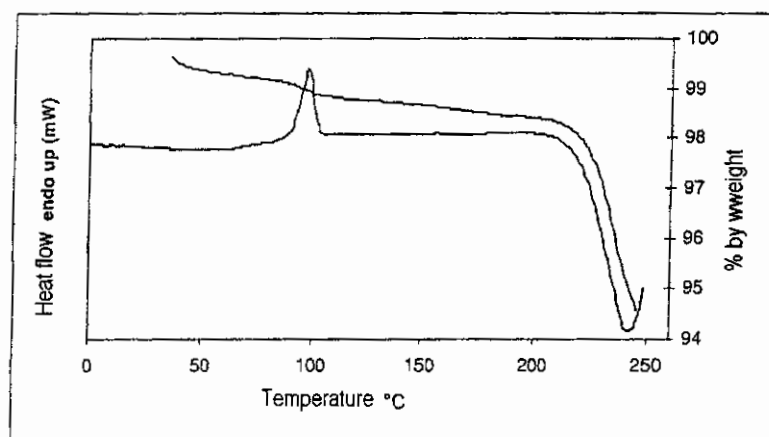


Figure 17

DSC and TGA thermograms of a sample of WX-671 (free base) crystallized from acetonitrile in the freezer

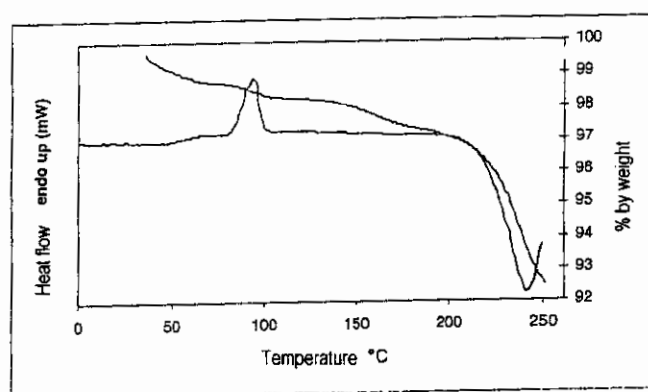


Figure 18

Micrograph of WX-671 after crystallization from acetonitrile in the freezer

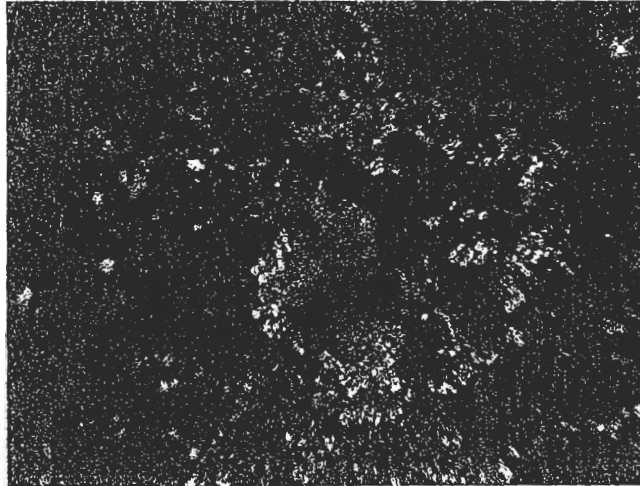


Figure 19

X-ray diffractogram of a sample of WX-671.1 (free base) crystallized from acetonitrile in the freezer

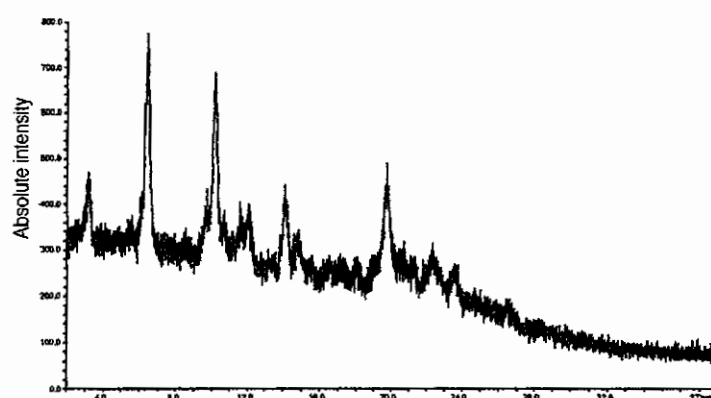


Figure 20

Sorption isotherm of water vapor on WX-671 at 22°C

