

FIGURES

Figure 1A

formula	C ₁₉ H ₂₄ N ₄ O ₇ S ₃
formula weight	516.62
Z, calculated density	2, 1.487 Mg · m ⁻³ .
F(000)	540
description and size of crystal	colorless plate, 0.02 · 0.13 · 0.15 mm ³
absorption coefficient	0.370 mm ⁻¹
min/max transmission	0.95/0.99
temperature	293K
radiation(wavelength)	Mo K α (λ = 0.71073 Å)
Crystal system, space group	triclinic, P -1
a	9.4908(7) Å
b	9.5545(7) Å
c	14.4137(9) Å
α	86.130(3)°
β	72.104(3)°
γ	68.253(4)°
V	1153.68(15) Å ³
min/max Θ	2.426° / 30.065°
number of collected reflections	43492
number of independent reflections	6761 (merging r = 0.026)
number of observed reflections	4955 ($I > 3.0\sigma(I)$)
number of refined parameters	298
r	0.0313 (observed data with)
R _W	0.0432 (all data)
goodness of fit	1.0736
residual electron density	-0.28/0.33 e Å ³

Figure 1 B
X-Ray Diffractogram of: BXR3NC1 calculated from single crystal data

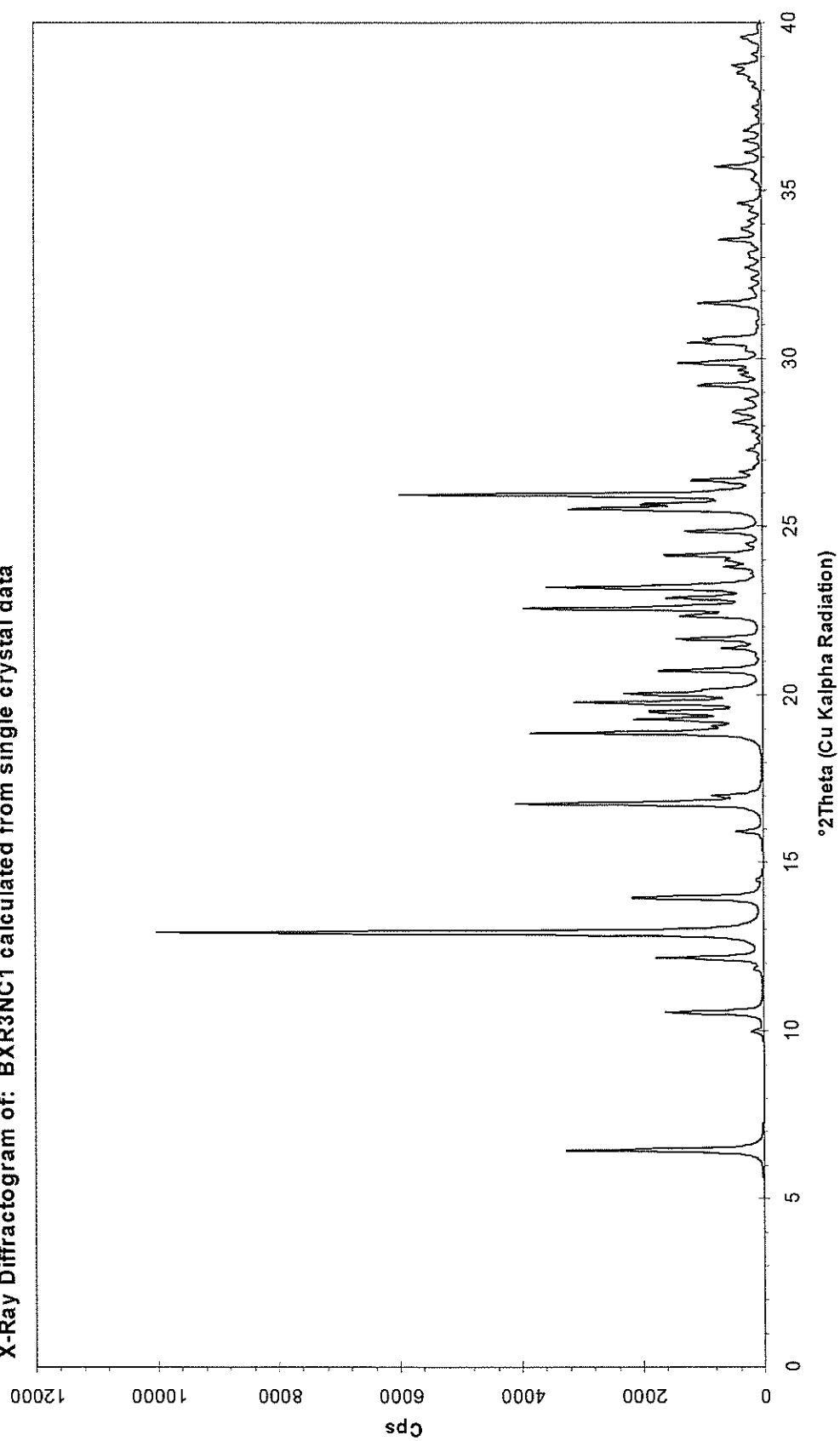


Figure 1C

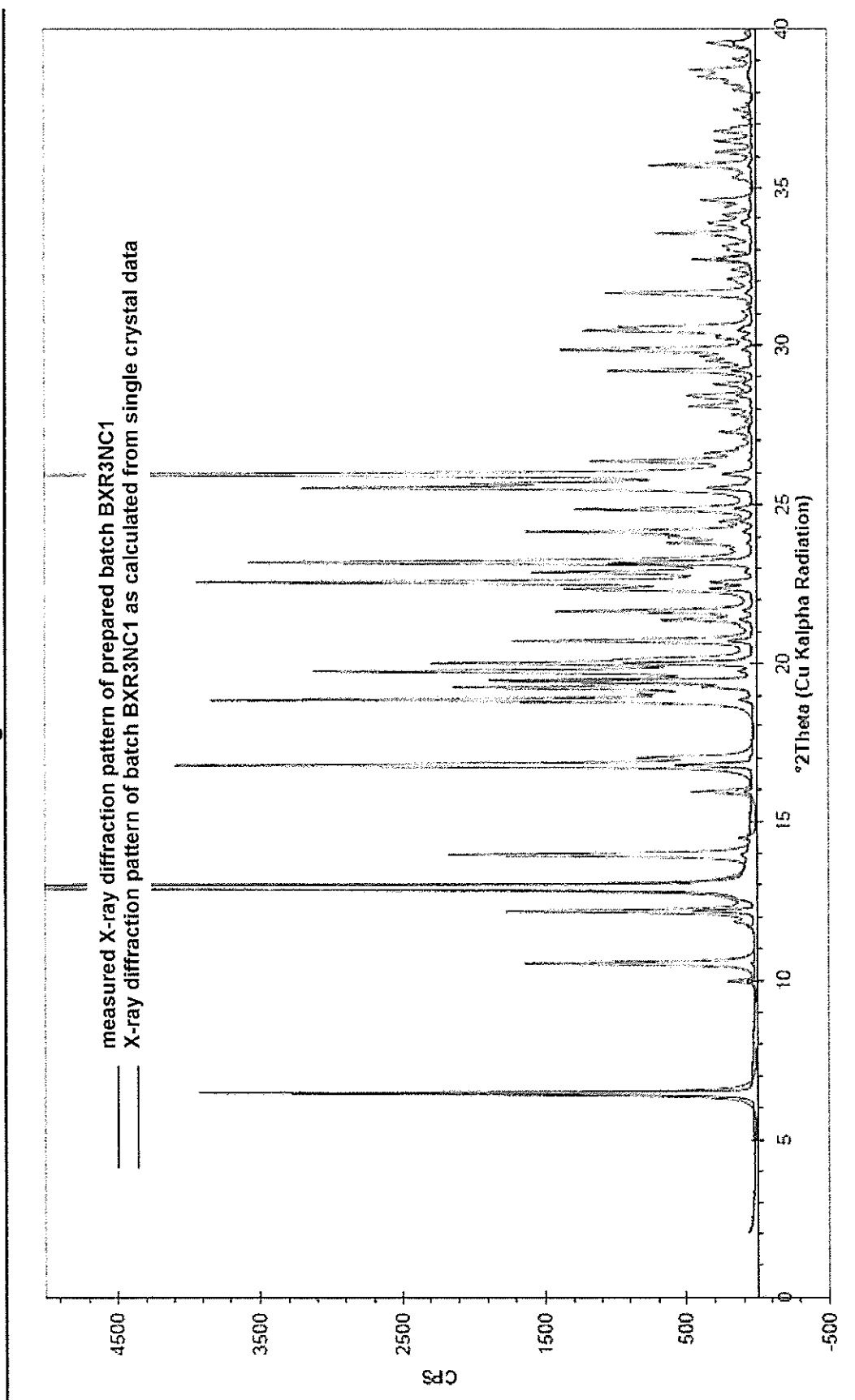


Figure 1D

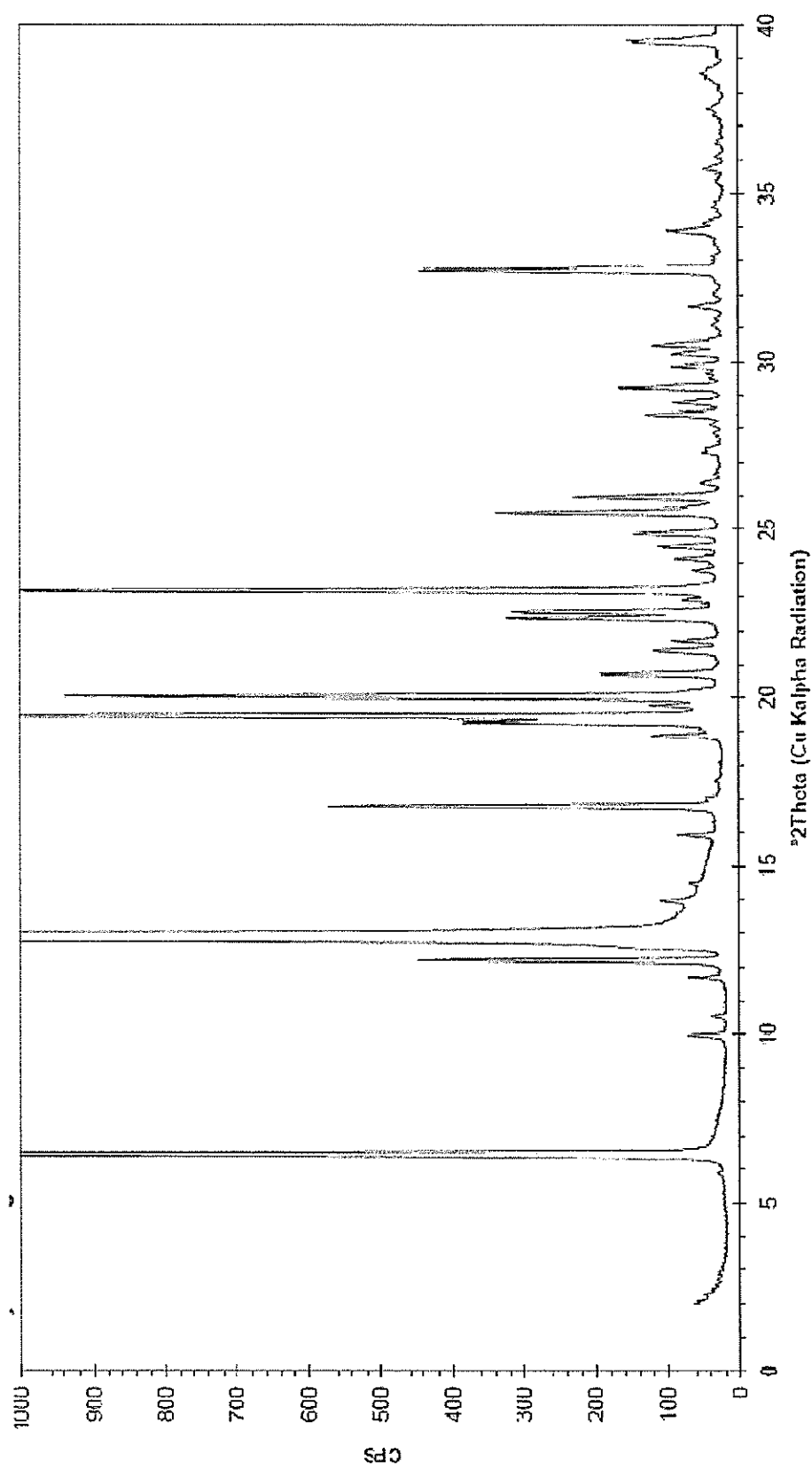
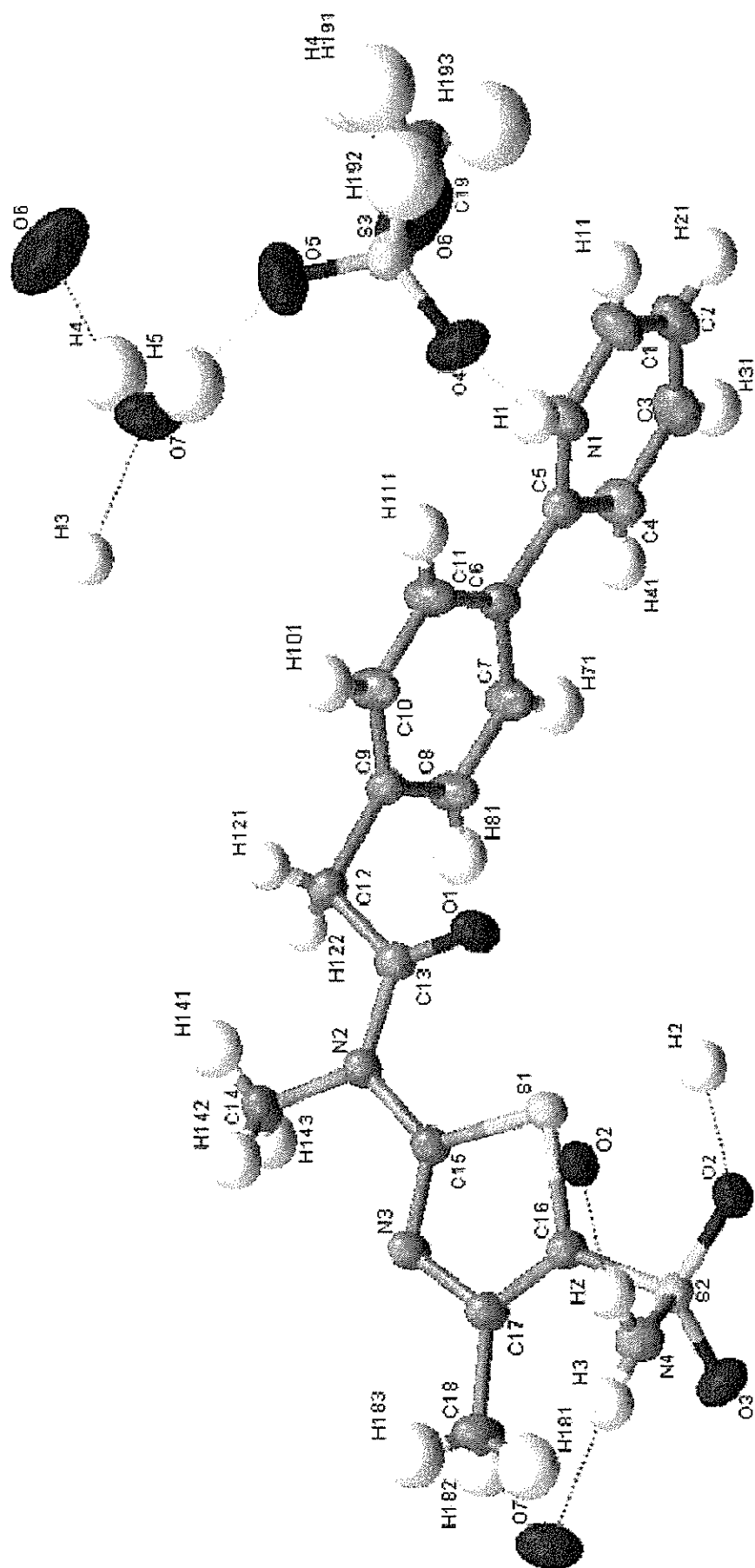


Figure 2



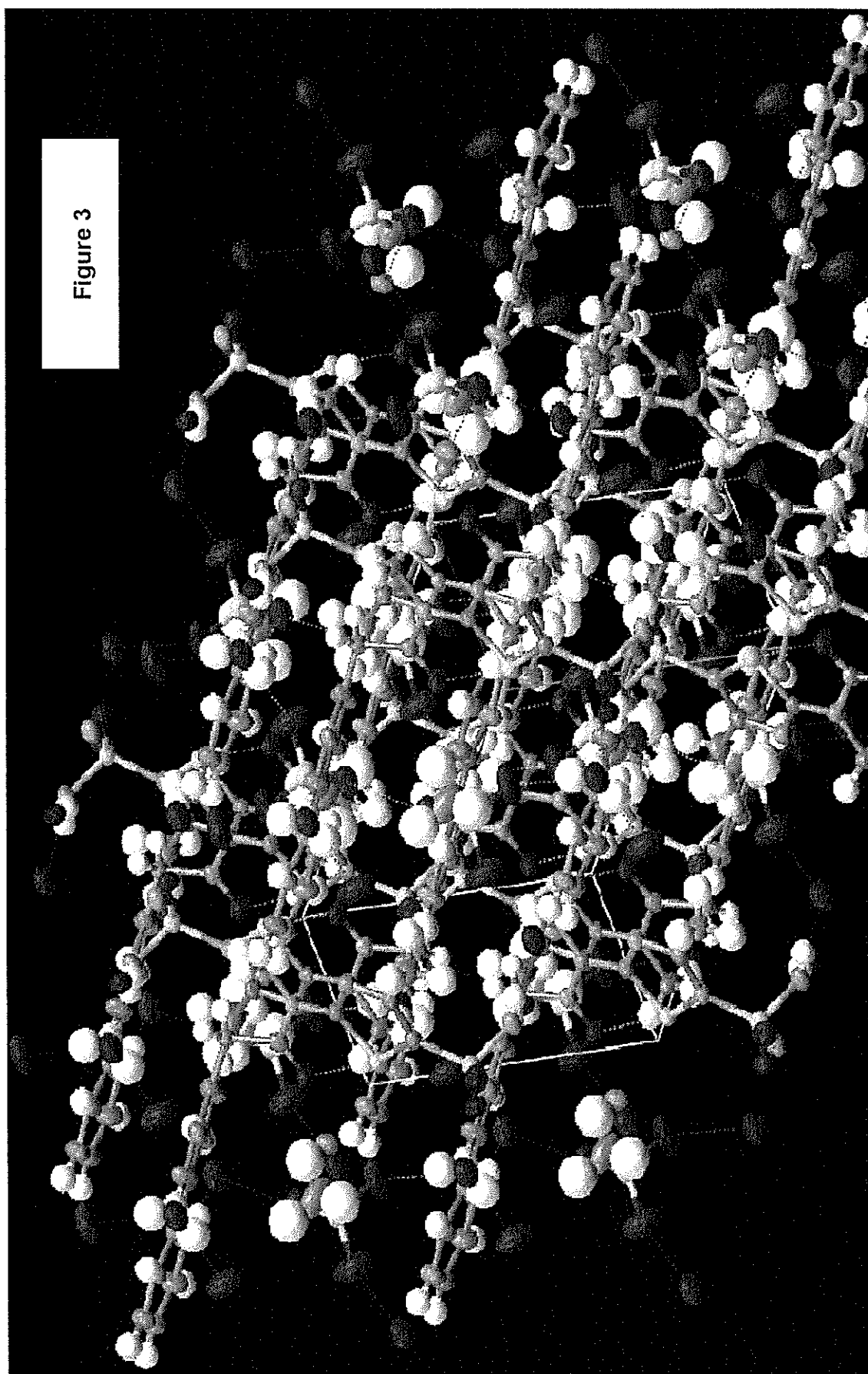


Figure 3