FIGURES

Figure 1A

formula	$C_{19}H_{24}N_4O_7S_3$
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 mm3
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 refections	6761 (merging r = 0.026)
number of observed reflections	4955 (I>3.0σ(I))
number of refined parameters	298
r	0.0313 (observed data with)
rW	0.0432 (all data)
goodness of fit	1.0736
residual electron density	-0.28/0.33 e $Å^3$

Figure 1 B

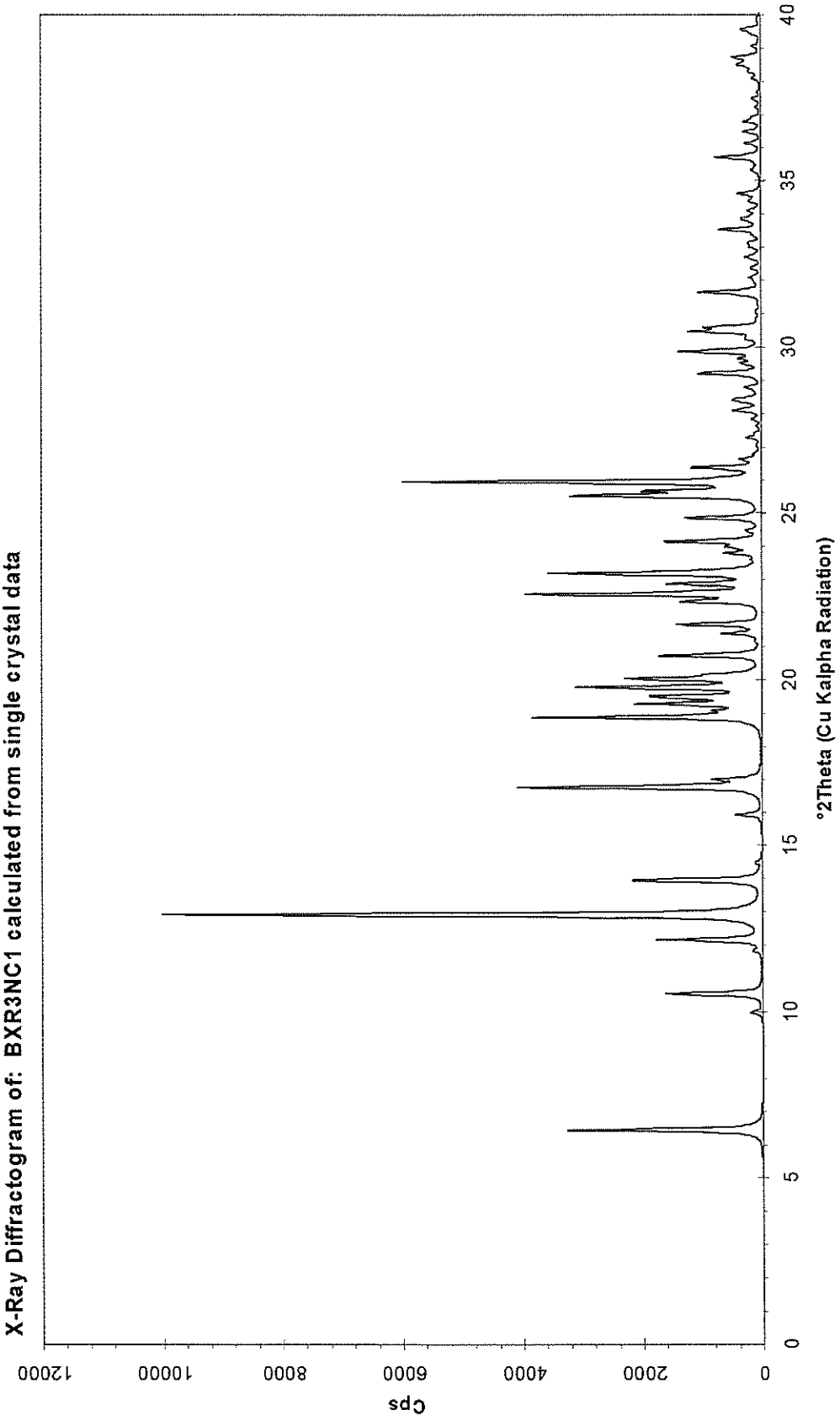

X-Ray Diffractogram of: BXR3NC1 calculated from single crystal data
Cps
0
2000
4000
6000
8000
10000
12000
0
5
10
15
20
25
30
35
40
°2Theta (Cu Kalpha Radiation)

Figure 1C

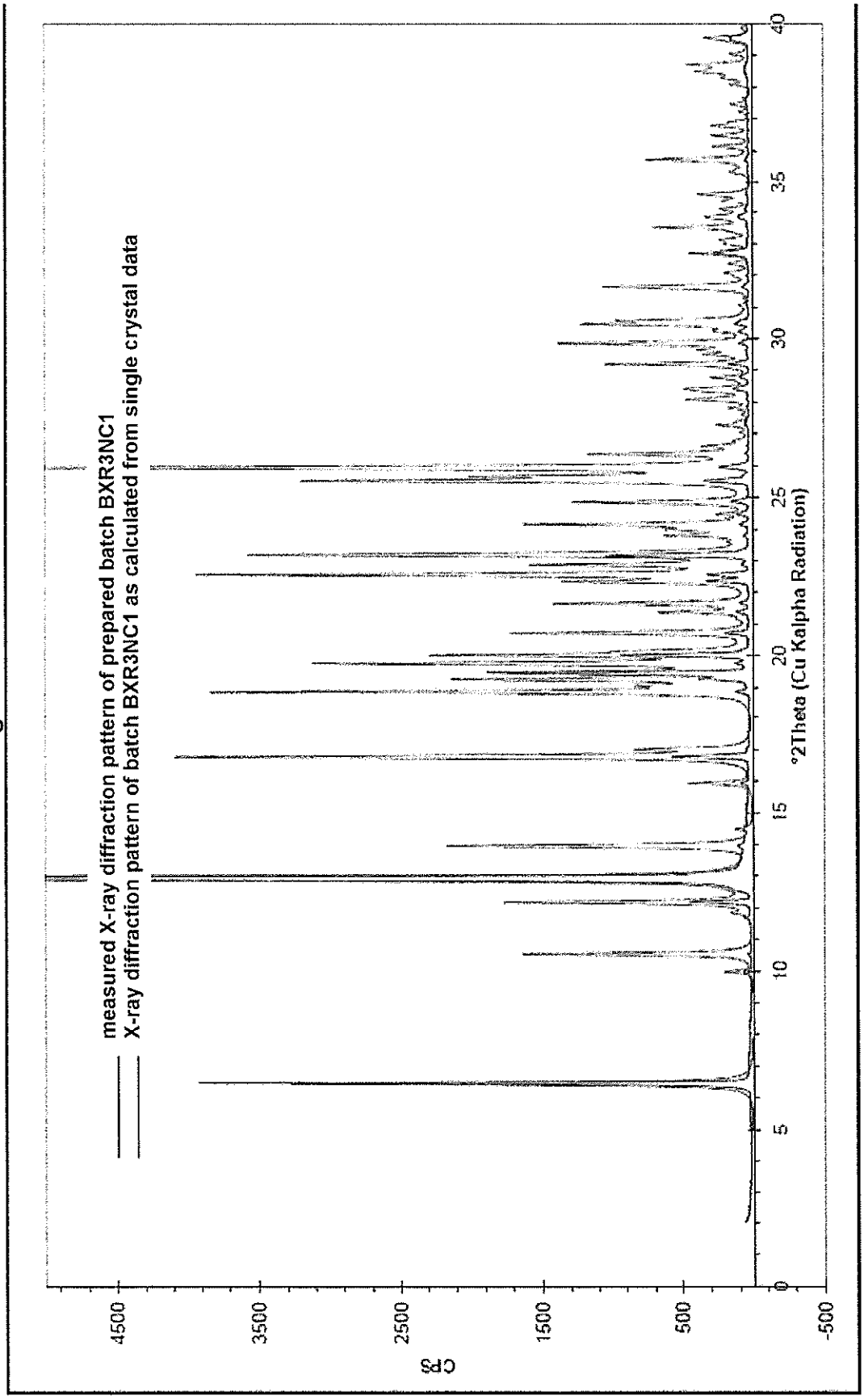

measured X-ray diffraction pattern of prepared batch BXR3NC1
X-ray diffraction pattern of batch BXR3NC1 as calculated from single crystal data
CPS
4500
3500
2500
1500
500
-500
0
5
10
15
20
25
30
35
40
°2Theta (Cu Kalpha Radiation)

Figure 1D

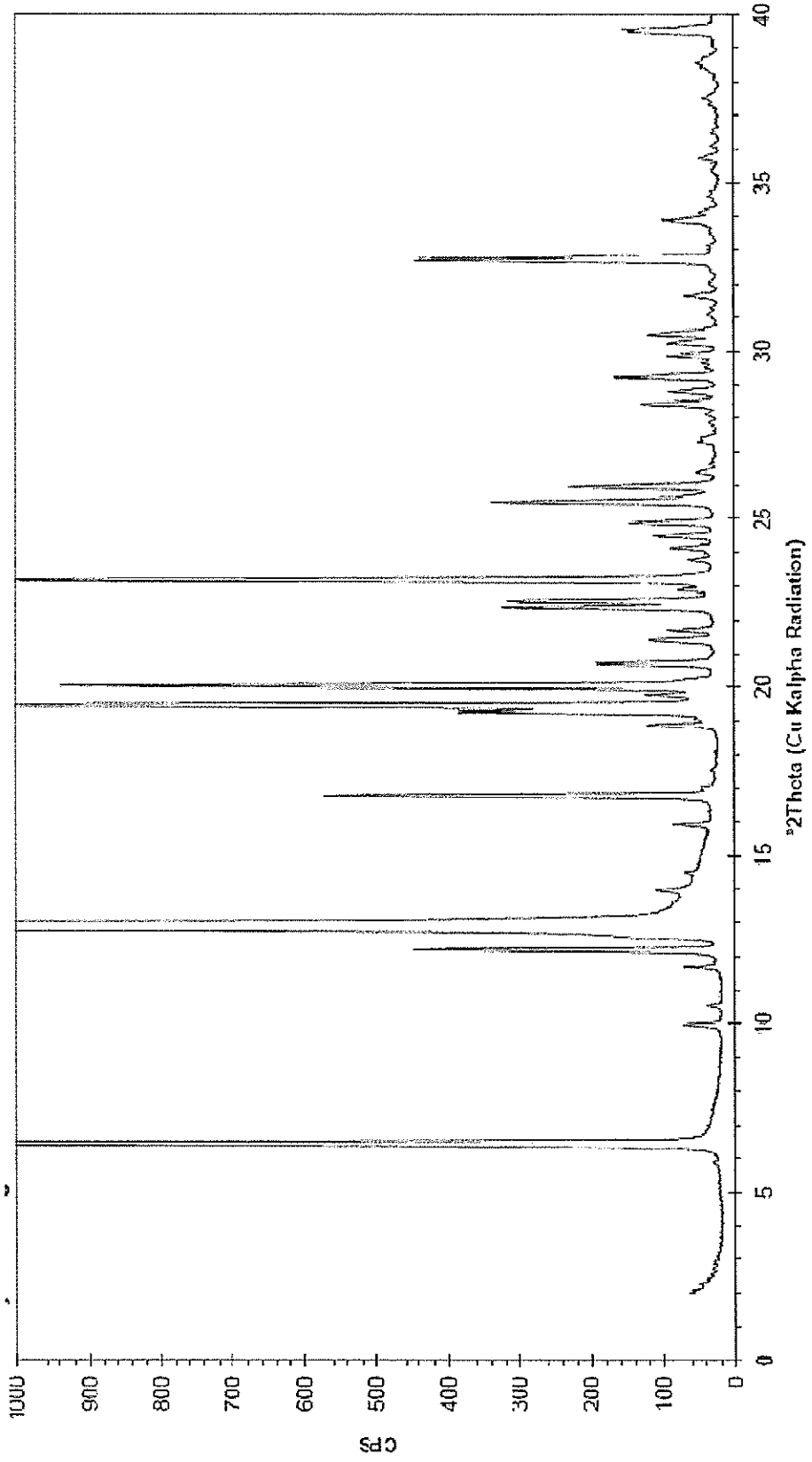
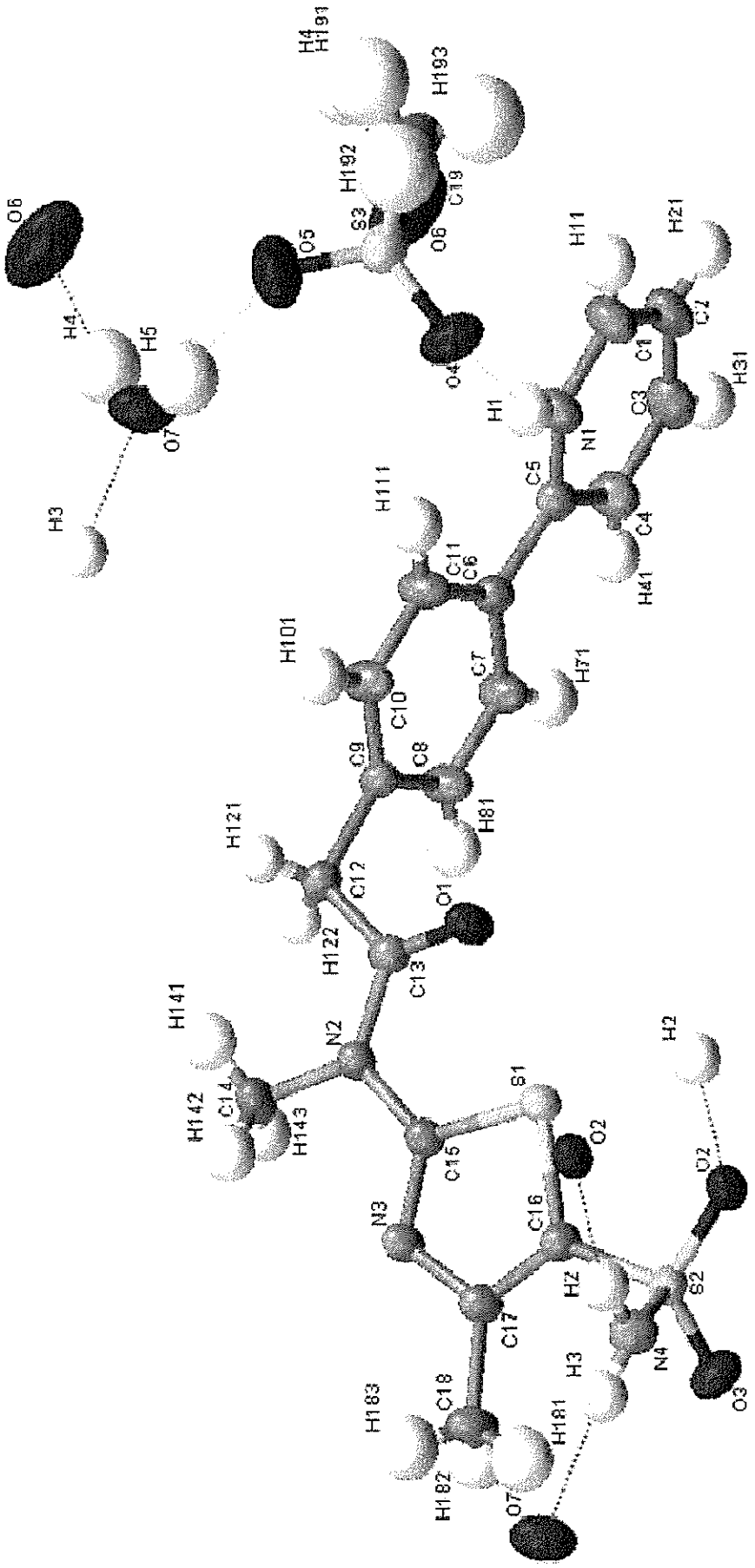

CPS
1000
900
800
700
600
500
400
300
200
100
0
0
5
10
15
20
25
30
35
40
°2Theta (Cu Kalpha Radiation)

Figure 2


O6
H4
H5
O7
H3
H4
H191
H193
H192
S3
C19
O5
O6
O4
H1
H11
H21
C2
C1
H31
O3
N1
C5
C4
H41
H111
C11
C6
H101
C10
C7
H71
C9
C8
H81
H121
C12
O1
H122
C13
H141
N2
C14
H142
H143
S1
O2
C15
N3
C16
H2
O2
S2
C17
N4
H3
O3
H183
C18
H181
H182
O7

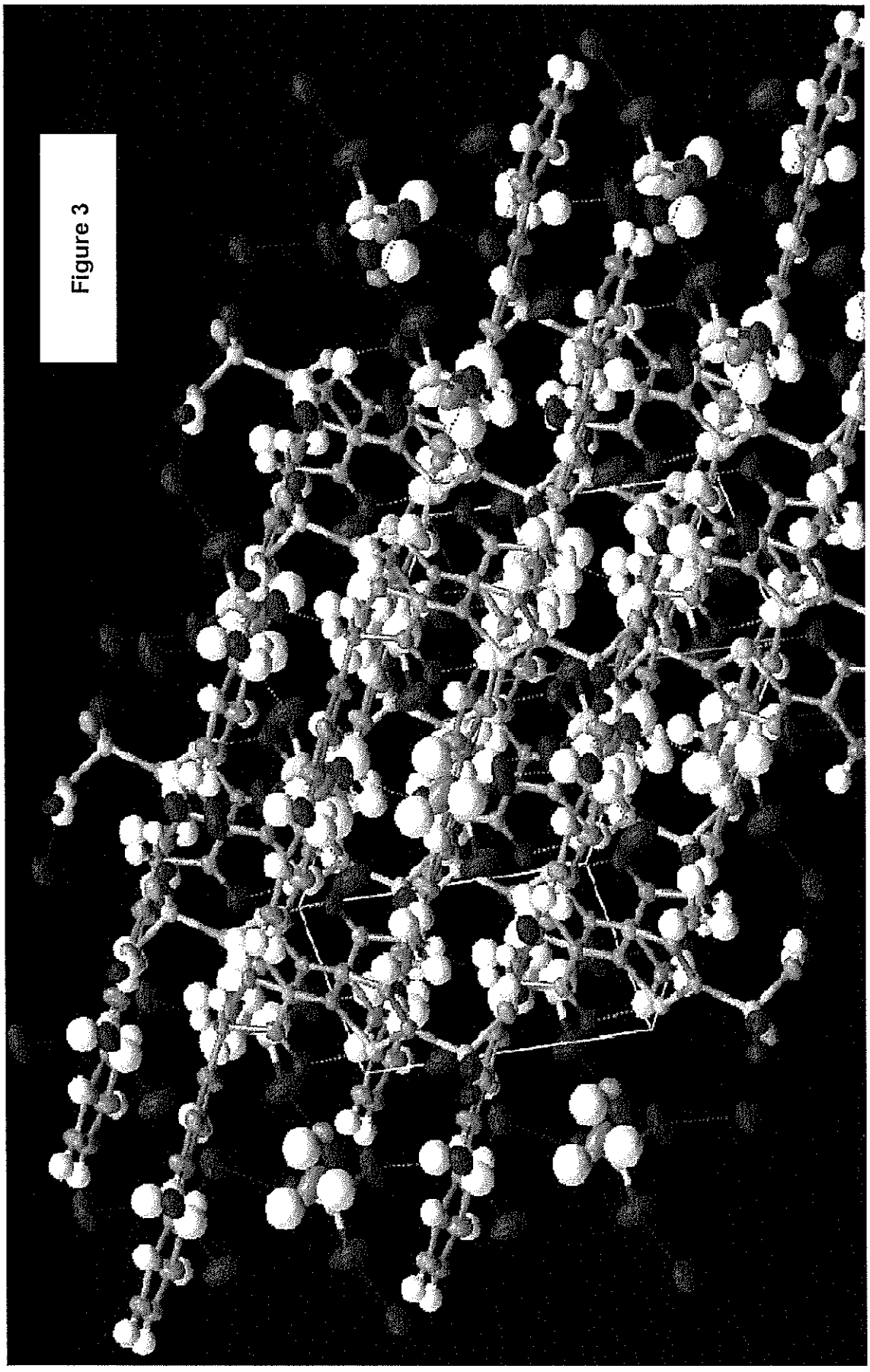


Figure 3