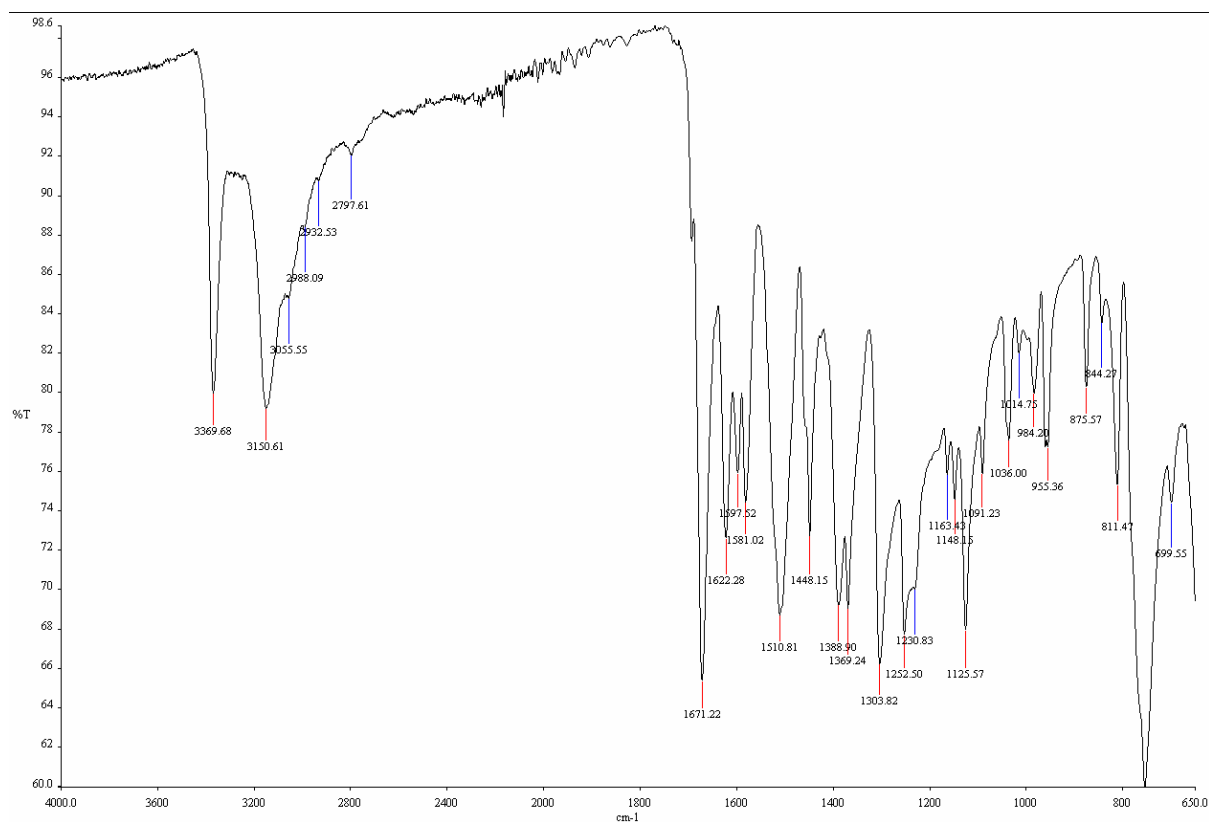
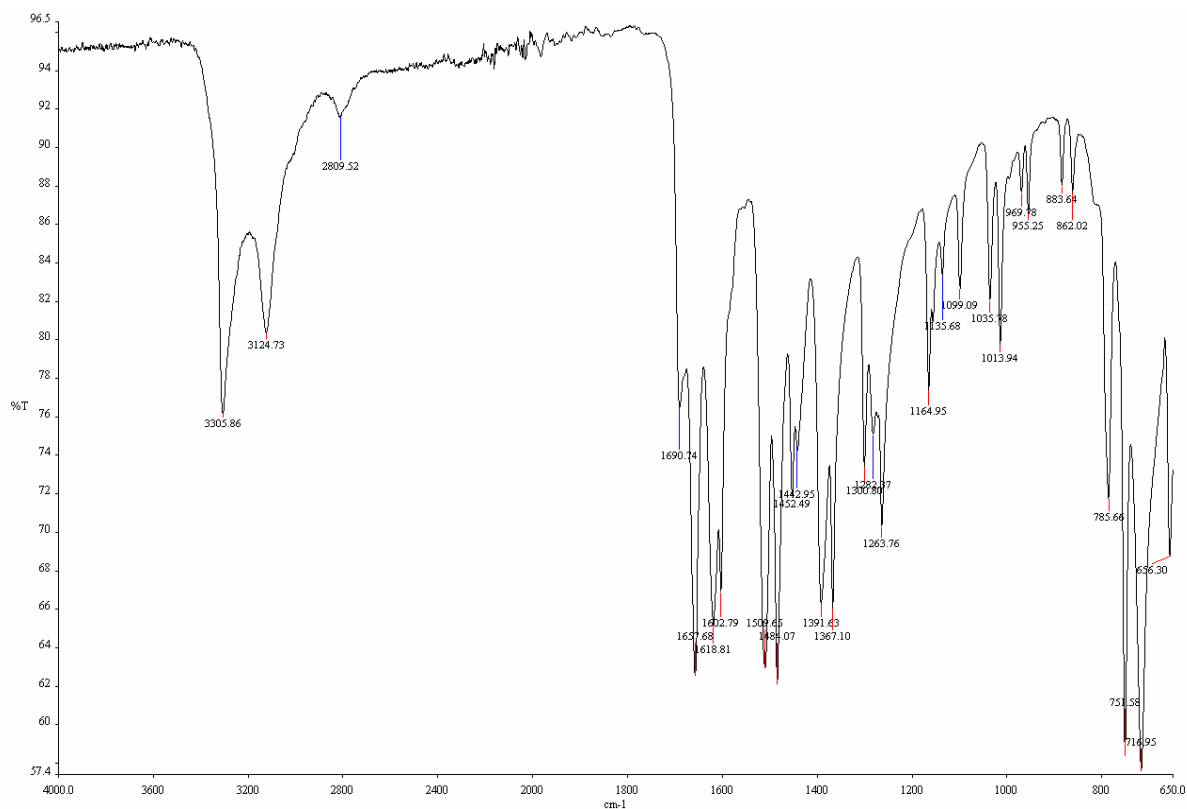


## The solvates of *o*-acetamidobenzamide

IR spectra collected using a PerkinElmer Spectrum One FT-IR ATR (diamond substrate) spectrometer over the range 650–4000  $\text{cm}^{-1}$  for crystals of the two polymorphs of AABA.

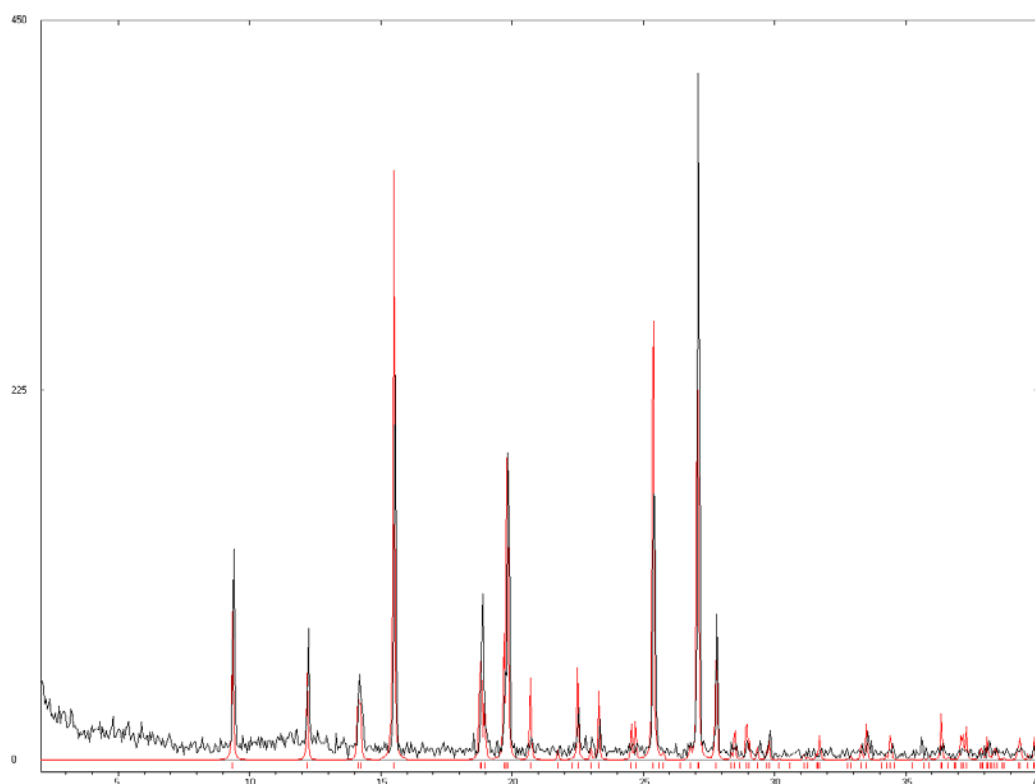


The IR spectrum observed for the  $\alpha$ -form of AABA

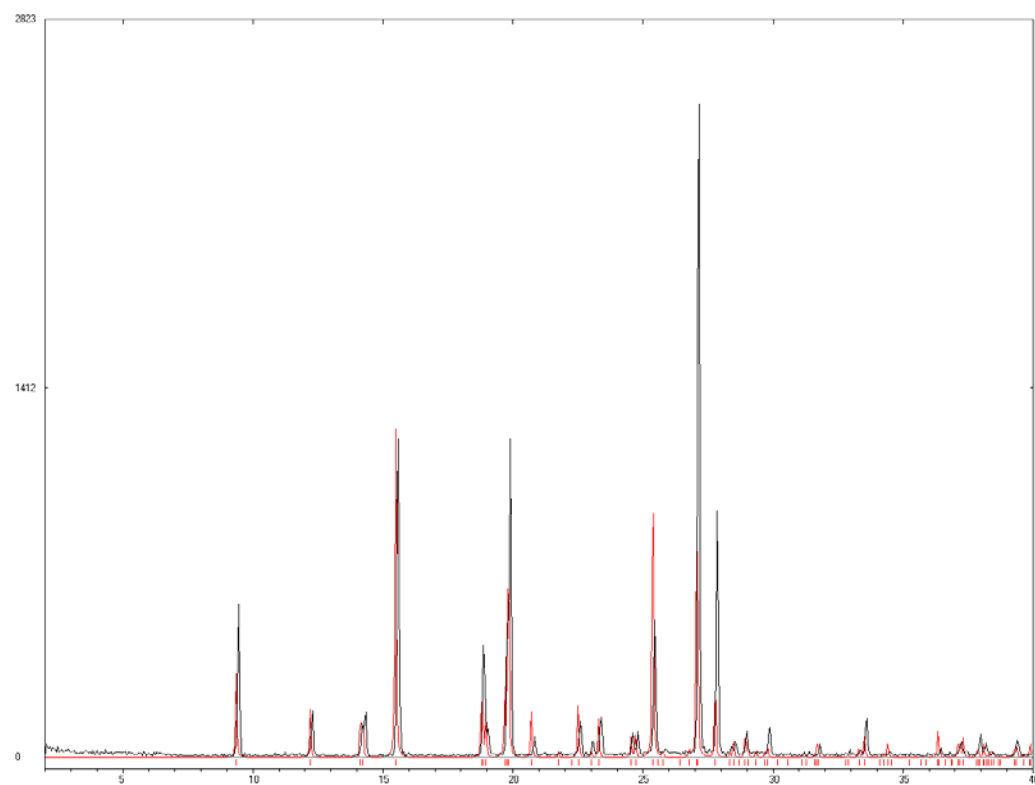


The IR spectrum observed for the  $\beta$ -form of AABA

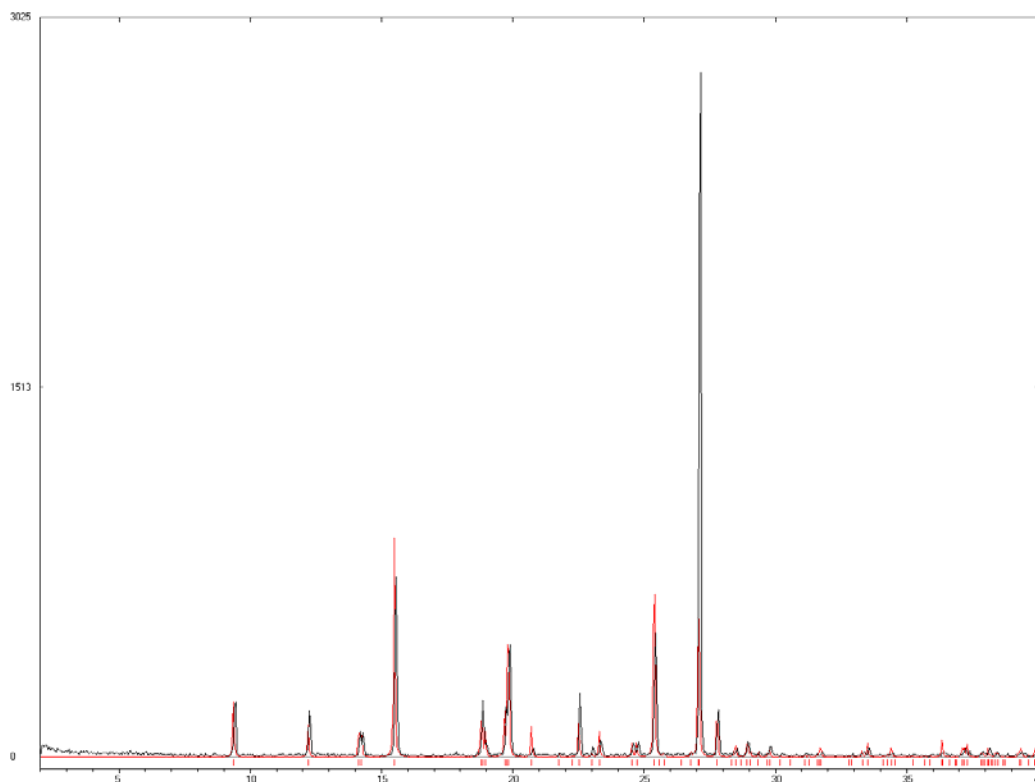
**Powder patterns for the other samples**



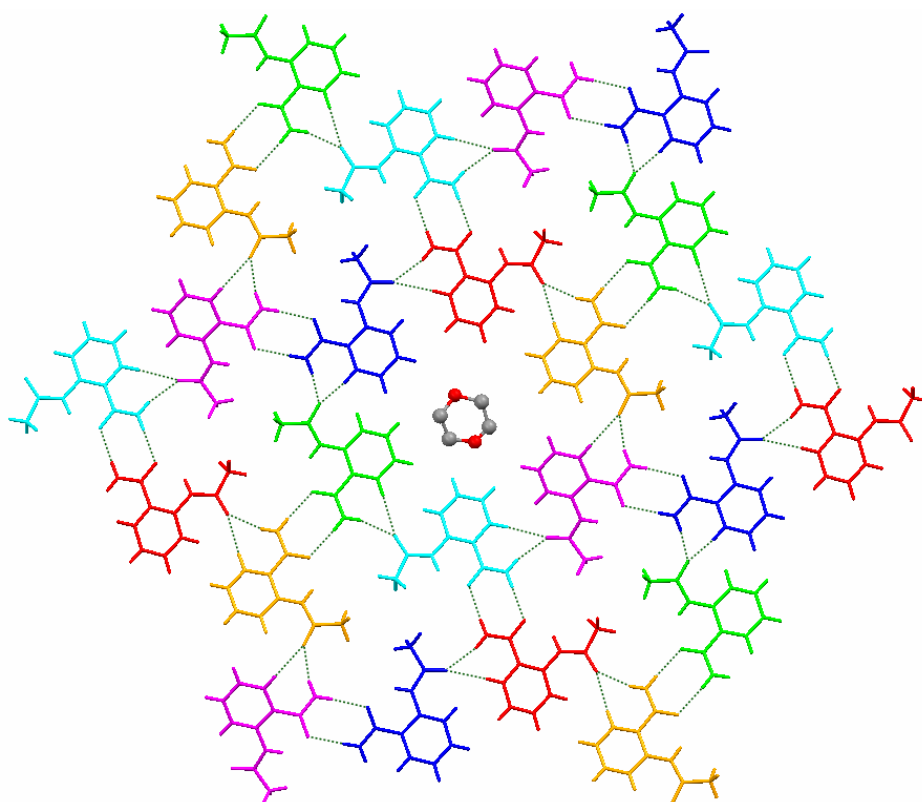
The observed powder pattern for the decomposition of [(AABA)<sub>6</sub>(1-PrOH)] (black line) compared with the calculated pattern for the α-form of AABA (red line).



The observed powder pattern for the decomposition of [(AABA)<sub>6</sub>(1-BuOH)] (black line) compared with the calculated pattern for the α-form of AABA (red line).



The observed powder pattern for the decomposition of  $[(AABA)_6(Diox)]$  (black line) compared with the calculated pattern for the  $\alpha$ -form of AABA (red line).



Part of the sheet formed by  $[(AABA)_6.Dioxane]$  showing the hydrogen-bonding interactions.

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 Hydrogen-bonding interactions for [(AABA)<sub>6</sub>.Dioxane].

	D-H/Å	D-H...A/Å	D...A/Å	D-H...A/°
N2-H2A...O1	0.88	1.97	2.645(7)	132.9
N12-H12A...O11	0.88	1.93	2.657(7)	139.1
N22-H22A...O21	0.88	1.97	2.635(9)	131.5
N32-H32A...O31	0.88	1.93	2.654(7)	138.3
N42-H42A...O41	0.88	1.90	2.630(6)	139.6
N52-H52A...O51	0.88	1.89	2.628(9)	140.3
N1-H1A...O31	0.88	2.09	2.964(7)	176.1
N1-H1B...O52 <sup>vii</sup>	0.88	2.15	3.002(9)	163.9
C3-H3A...O52 <sup>vii</sup>	0.95	2.39	3.336(11)	172.0
N11-H11A...O41 <sup>viii</sup>	0.88	2.05	2.929(8)	177.0
N11-H11B...O2 <sup>ix</sup>	0.88	2.05	2.896(9)	161.7
C13-H13A...O2 <sup>ix</sup>	0.95	2.45	3.188(8)	134.8
N21-H21A...O51	0.88	2.06	2.944(9)	177.2
N21-H21B...O12 <sup>x</sup>	0.88	2.12	2.975(7)	164.6
C23-H23A...O12 <sup>x</sup>	0.95	2.48	3.308(9)	145.2
N31-H31A...O1	0.88	2.10	2.979(7)	172.3
N31-H31B...O22	0.88	2.09	2.951(9)	165.4
C33-H33A...O22	0.95	2.34	3.270(10)	167.4
N41-H41A...O11 <sup>viii</sup>	0.88	2.10	2.976(8)	175.3
N41-H41B...O32 <sup>xi</sup>	0.88	2.07	2.929(8)	163.8
C43-H43A...O32 <sup>xi</sup>	0.95	2.53	3.309(7)	139.6
N51-H51A...O21	0.88	2.04	2.925(9)	179.3
N51-H51B...O42 <sup>xii</sup>	0.88	2.13	2.987(7)	163.2
C53-H53A...O42 <sup>xii</sup>	0.95	2.35	3.300(10)	174.4

Symmetry operations for equivalent atoms

vii =  $x-1, y-1, z$ ; viii =  $-x+1, -y+1, -z+1$ ; ix =  $x, y, z+1$ ; x =  $x+1, y, z$ ; xi =  $-x+1, -y, -z+1$ ; xii =  $-x+1, -y+1, -z$ .