Chains or Rings? Polymorphism of an isoniazid derivative derivatized with diacetone alcohol

Matthew C. Scheepers and Andreas Lemmerer*‡

Supplementary Information

1. **Table S1** Crystallographic information for the crystal structures of **Form I** and **Form II**

Crystal Form	**Form I**	**Form II**
Empirical formula	$C_{12}H_{17}N_3O_2$	$C_{12}H_{17}N_3O_2$
Formula weight	235.28	235.28
Temperature/K	173(2)	173(2)
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/c	$P2_1/c$
a/Å	21.8108(4)	9.2041(2)
b/Å	7.0776(2)	11.1274(3)
c/Å	18.1625(5)	11.9383(3)
α/°	90	90
β/°	116.465(3)	92.3570(10)
γ/°	90	90
Volume/Å^3	2509.90(12)	1221.66(5)
Z	8	4
Density/ g/cm^3	1.245	1.279
μ/mm-1	0.087	0.089
F(000)	1008	504
Crystal size/mm^3	0.255 x 0.184 x 0.152	0.728 x 0.495 x 0.228

2Θ range for data collection/°	2.086 to 28.420	2.215 to 28.330
Reflections collected	37052	50485
Independent reflections	3065 [R(int) = 0.1191]	3029 [R(int) = 0.0395]
Goodness-of-fit on F^2	0.863	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.0978	R_1 = 0.0382, wR_2 = 0.0896
Final R indexes [all data]	R_1 = 0.0933, wR_2 = 0.1115	R_1 = 0.0578, wR_2 = 0.0987
CCDC	2133557	2133558

2. PXRD patterns

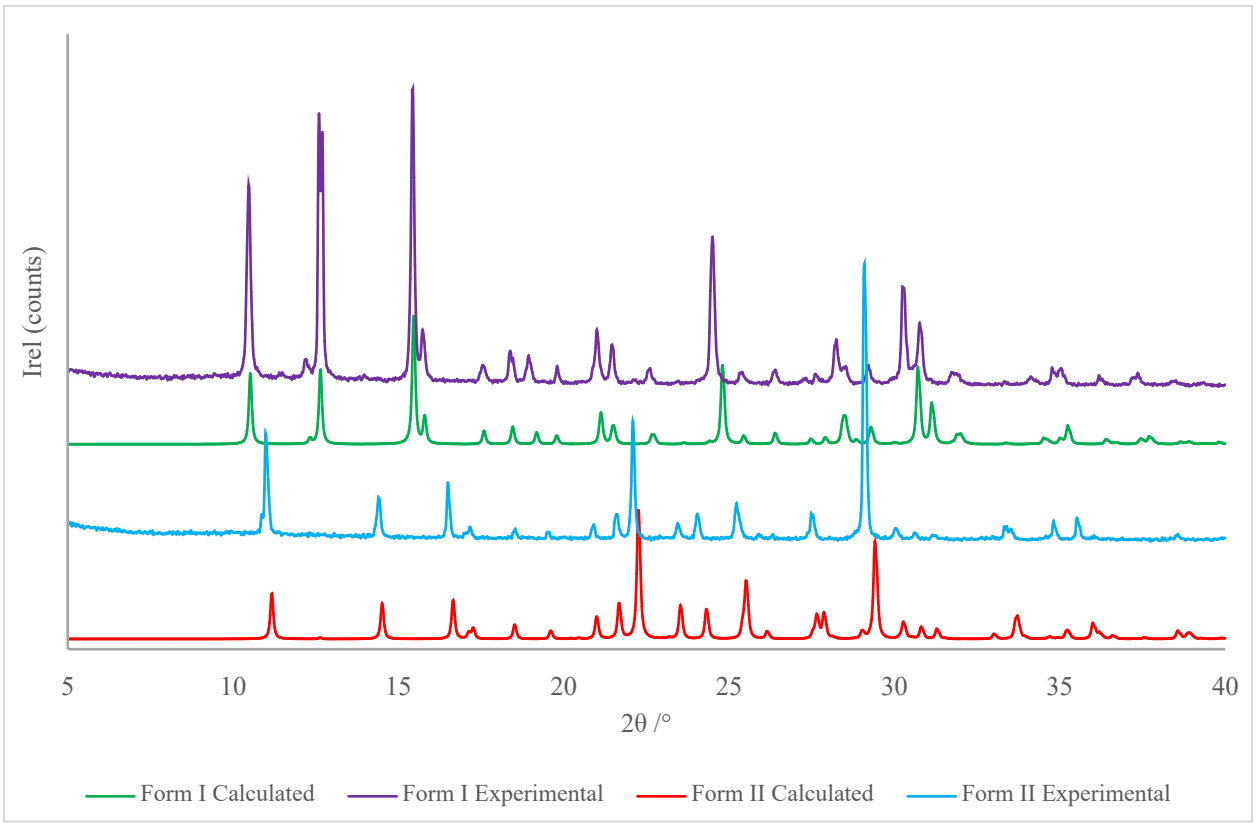

Figure S1 PXRD Patterns for both **Form I** and **Form II,** calculated and experimental.

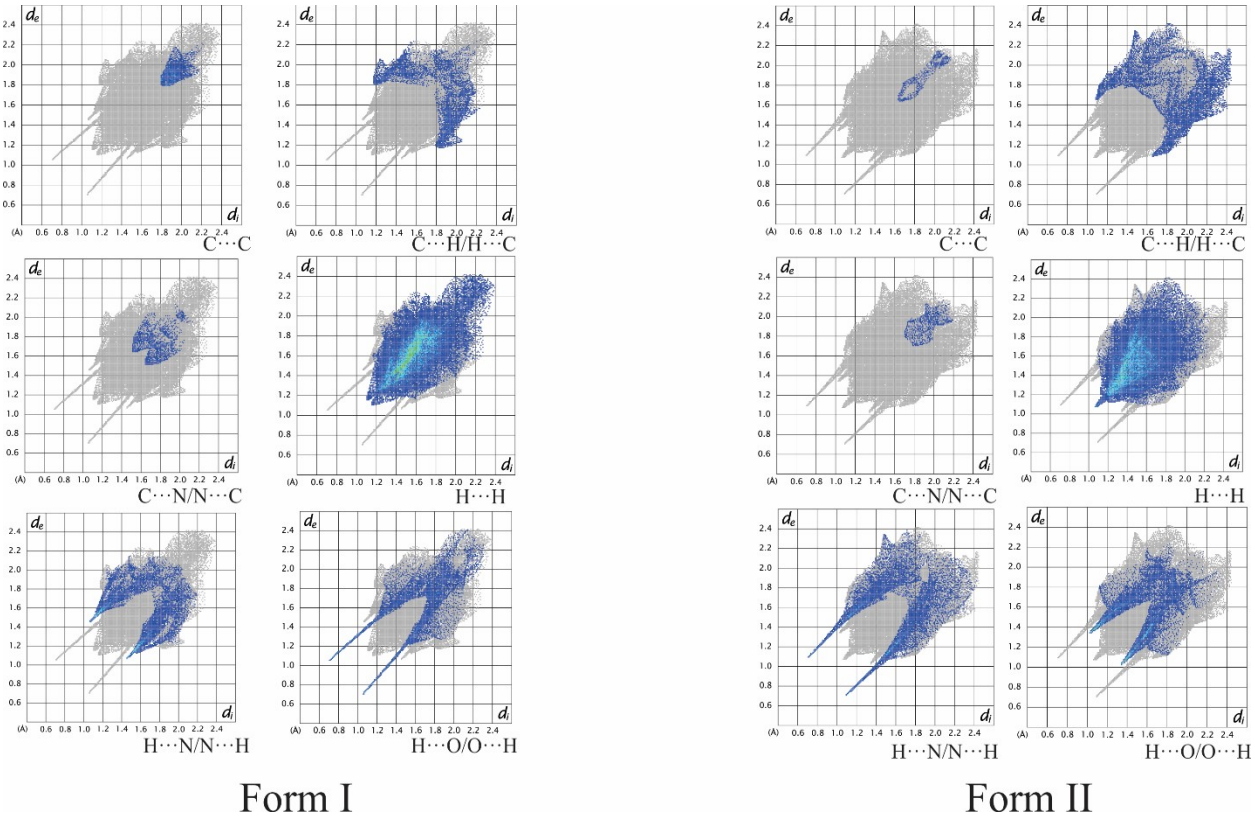

Figure S2 Hirshfeld Surface Fingerprint spots for both **Form I** and **Form II**