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Supporting information for article:

Two conformational polymorphs of 4-methylhippuric acid

Marilia Guillén, Asiloé J. Mora, Lusbely M. Belandria, Luis E. Seijas, Jeans W. Ramírez, José L. Burgos, Luis Rincón and Gerzon E. Delgado

Supporting information

Table S1 Assignment of IR absorption bands for polymorphs I and II of 4-methylhippuric acid.

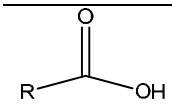
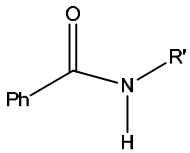
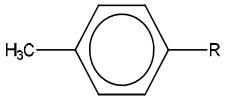
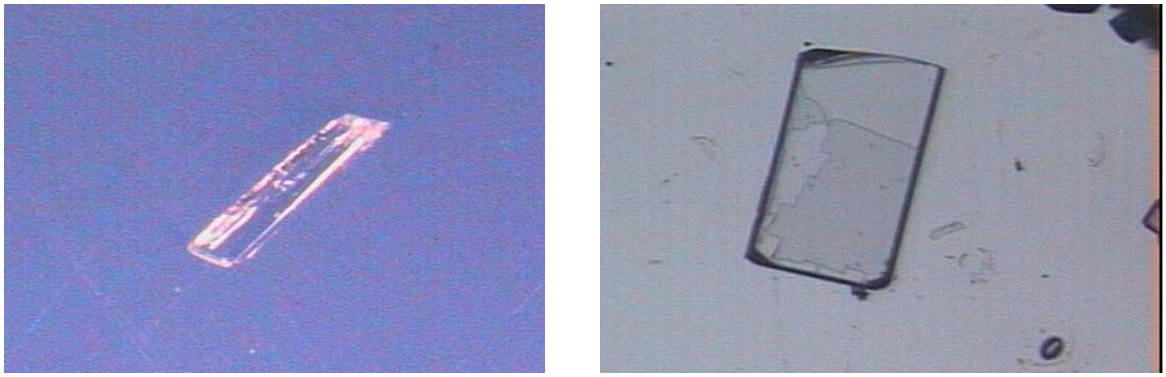
Functional group	**Bond type**	**Type of vibration**	**Wave number, υ (cm^{-1})**	
			Polymorph I	*Polymorph II*
	O—H	Stretching	3200-2750	3138-2770
			1396, 1418	1395, 1387, 1422, 1419
	C=O	Stretching	1741	1748, 1734
	C—O	Stretching	1218	1218
	N—H	Stretching	3354	3354
		Bending	1522	1522, 1516
		Deformation	756	755
	C=O	Stretching	1653, 1616	1653, 1647, 1623, 1616
	C—N	Stretching	1457	1457
	$H-C_{sp^2}$	Stretching	3048	3050
		Bending	832	833
	C=C	Stretching	1559	1559, 1540
	$H-C_{sp^3}$	Stretching	2987	2987
	C—C	Stretching	1023	1023
$-CH_2-$	C—H	Stretching	2933	2932

Table S2 Selected geometric parameters (Å, º)

4MH-I			
O1—C1	1.317 (4)	C4—C9	1.389 (4)
O2—C1	1.198 (4)	C5—C6	1.376 (4)
O3—C3	1.229 (4)	C6—C7	1.382 (5)
N1—C3	1.344 (5)	C7—C8	1.374 (4)
N1—C2	1.431 (5)	C7—C10	1.512 (4)
C1—C2	1.497 (5)	C8—C9	1.380 (4)
C3—C4	1.470 (5)	O1—H1	0.840 (4)
C4—C5	1.388 (4)	N1—H4	0.820 (4)
C3—N1—C2	122.6 (4)	C3—N1—H4	115 (3)
O2—C1—O1	123.9 (3)	C9—C4—C3	124.5 (3)
O2—C1—C2	125.8 (3)	C6—C5—C4	121.4 (3)
O1—C1—C2	110.4 (4)	C5—C6—C7	121.0 (3)
N1—C2—C1	113.4 (3)	C8—C7—C6	117.9 (3)
O3—C3—N1	119.9 (4)	C8—C7—C10	120.8 (4)
O3—C3—C4	121.6 (4)	C6—C7—C10	121.3 (3)
N1—C3—C4	118.5 (4)	C7—C8—C9	121.6 (3)
C5—C4—C9	117.4 (3)	C8—C9—C4	120.6 (3)
C5—C4—C3	118.1 (4)	C1—O1—H1	111 (2)
C2—N1—H4	123 (3)		
C3—N1—C2—C1	-83.5(5)	C9—C4—C5—C6	2.3(5)
C2—N1—C3—O3	2.1(6)	C3—C4—C9—C8	177.5(3)
C2—N1—C3—C4	-176.4(4)	C5—C4—C9—C8	-2.3(5)
O1—C1—C2—N1	169.9(3)	C4—C5—C6—C7	-1.1(5)
O2—C1—C2—N1	-11.1(5)	C5—C6—C7—C8	-0.1(5)
O3—C3—C4—C5	-8.6(6)	C5—C6—C7—C10	179.7(3)
O3—C3—C4—C9	171.7(4)	C6—C7—C8—C9	0.1(5)
N1—C3—C4—C5	169.8(4)	C10—C7—C8—C9	-179.8(3)
N1—C3—C4—C9	-9.9(6)	C7—C8—C9—C4	1.2(5)
C3—C4—C5—C6	-177.5(3)		
4MH-II			
O1A—C1A	1.326 (2)	O1B—C1B	1.319 (2)
O2A—C1A	1.205 (2)	O2B—C1B	1.206 (2)

O3A—C3A	1.238 (2)	O3B—C3B	1.241 (2)
N1A—C3A	1.338 (3)	N1B—C3B	1.340 (3)
N1A—C2A	1.442 (3)	N1B—C2B	1.445 (2)
C1A—C2A	1.506 (3)	C1B—C2B	1.493 (3)
C3A—C4A	1.490 (3)	C3B—C4B	1.490 (3)
C4A—C9A	1.379 (3)	C4B—C9B	1.382 (3)
C4A—C5A	1.391 (3)	C4B—C5B	1.388 (3)
C5A—C6A	1.376 (3)	C5B—C6B	1.382 (3)
C6A—C7A	1.374 (3)	C6B—C7B	1.374 (3)
C7A—C8A	1.383 (3)	C7B—C8B	1.381 (3)
C7A—C10A	1.514 (3)	C7B—C10B	1.519 (3)
C8A—C9A	1.381 (3)	C8B—C9B	1.384 (3)
O1A—H1A	0.910 (3)	O1B—H1B	0.860 (3)
N1A—H4A	0.850 (2)	N1B—H4B	0.862 (2)
C3A—N1A—C2A	120.61 (19)	C3B—N1B—C2B	121.50 (18)
O2A—C1A—O1A	124.58 (18)	O2B—C1B—O1B	124.74 (19)
C1A—O1A—H1A	109.7 (2)	O2B—C1B—C2B	124.81 (18)
O2A—C1A—C2A	124.29 (18)	O1B—C1B—C2B	110.45 (18)
O1A—C1A—C2A	111.13 (18)	N1B—C2B—C1B	114.32 (16)
N1A—C2A—C1A	112.87 (17)	O3B—C3B—N1B	121.14 (18)
C2A—N1A—H4A	119.5 (2)	O3B—C3B—C4B	120.57 (18)
C3A—N1A—H4A	119.8 (2)	N1B—C3B—C4B	118.19 (17)
O3A—C3A—N1A	119.9 (2)	C9B—C4B—C5B	117.79 (18)
O3A—C3A—C4A	120.85 (19)	C9B—C4B—C3B	124.24 (19)
N1A—C3A—C4A	119.20 (18)	C5B—C4B—C3B	117.94 (18)
C9A—C4A—C5A	117.2 (2)	C6B—C5B—C4B	121.1 (2)
C9A—C4A—C3A	124.61 (19)	C7B—C6B—C5B	121.6 (2)
C5A—C4A—C3A	118.21 (19)	C6B—C7B—C8B	117.0 (2)
C6A—C5A—C4A	121.6 (2)	C6B—C7B—C10B	120.4 (2)
C7A—C6A—C5A	121.6 (2)	C8B—C7B—C10B	122.5 (2)
C6A—C7A—C8A	116.8 (2)	C7B—C8B—C9B	122.3 (2)
C6A—C7A—C10A	121.2 (2)	C4B—C9B—C8B	120.2 (2)
C8A—C7A—C10A	122.1 (2)	C1B—O1B—H1B	111.0 (2)
C9A—C8A—C7A	122.4 (2)	C2B—N1B—H4B	119.4 (1)
C4A—C9A—C8A	120.6 (2)	C3B—N1B—H4B	118.8 (1)
C3A—N1A—C2A—C1A	-68.6(2)	C3B—N1B—C2B—C1B	77.7(2)

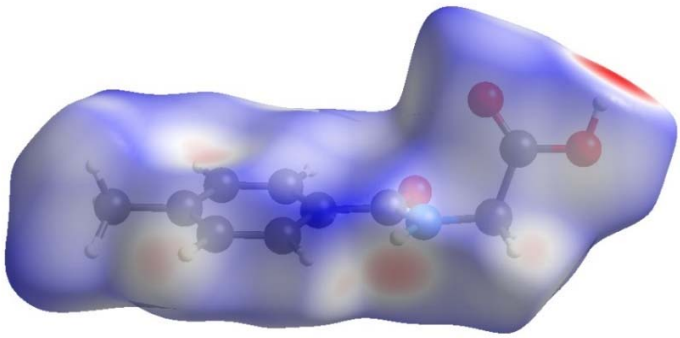
C2A—N1A—C3A—O3A	-1.9(3)	C2B—N1B—C3B—O3B	-5.8(3)
C2A—N1A—C3A—C4A	178.51(16)	C2B—N1B—C3B—C4B	170.64(16)
O1A—C1A—C2A—N1A	168.27(16)	O1B—C1B—C2B—N1B	-174.70(16)
O2A—C1A—C2A—N1A	-12.0(3)	O2B—C1B—C2B—N1B	5.0(3)
O3A—C3A—C4A—C5A	2.4(3)	O3B—C3B—C4B—C5B	29.1(3)
O3A—C3A—C4A—C9A	-178.79(19)	O3B—C3B—C4B—C9B	-153.17(19)
N1A—C3A—C4A—C5A	-178.05(18)	N1B—C3B—C4B—C5B	-147.35(18)
N1A—C3A—C4A—C9A	0.8(3)	N1B—C3B—C4B—C9B	30.4(3)
C3A—C4A—C5A—C6A	178.0(2)	C3B—C4B—C5B—C6B	176.53(18)
C9A—C4A—C5A—C6A	-0.9(3)	C9B—C4B—C5B—C6B	-1.4(3)
C3A—C4A—C9A—C8A	-178.7(2)	C3B—C4B—C9B—C8B	-177.48(18)
C5A—C4A—C9A—C8A	0.2(3)	C5B—C4B—C9B—C8B	0.3(3)
C4A—C5A—C6A—C7A	0.6(4)	C4B—C5B—C6B—C7B	1.4(3)
C5A—C6A—C7A—C8A	0.4(4)	C5B—C6B—C7B—C8B	-0.4(3)
C5A—C6A—C7A—C10A	-178.7(2)	C5B—C6B—C7B—C10B	179.1(2)
C6A—C7A—C8A—C9A	-1.2(4)	C6B—C7B—C8B—C9B	-0.8(3)
C10A—C7A—C8A—C9A	177.9(2)	C10B—C7B—C8B—C9B	179.8(2)
C7A—C8A—C9A—C4A	0.9(4)	C7B—C8B—C9B—C4B	0.8(3)



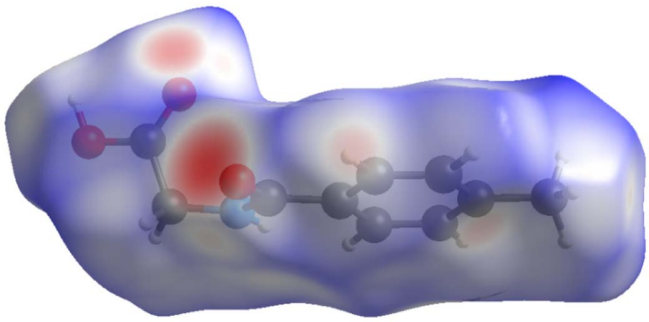
(a) (b)

Figure S1 Photographs of the crystals: (a) Polymorph **I** and (b) Polymorph **II**, taken from a Nikon polarized light Microscope.

(a)



(b)



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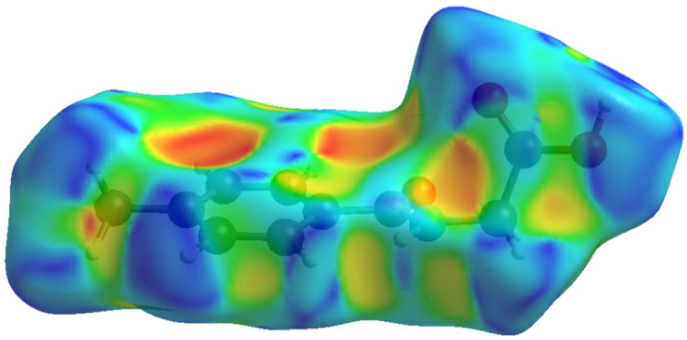


(d)

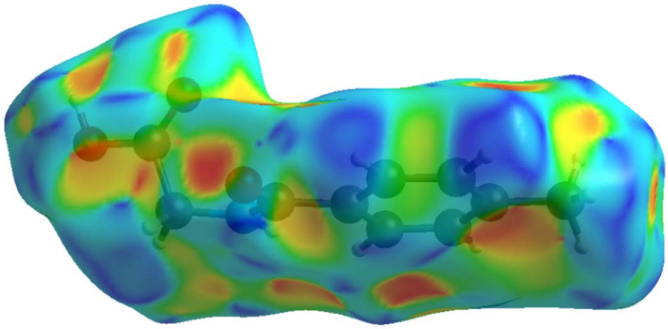
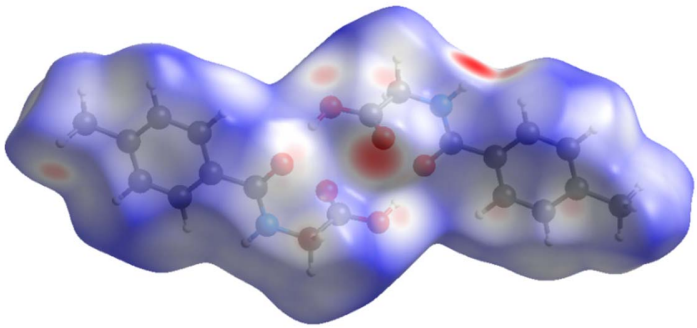


Figure S2 Views of Hirshfeld surface to polymorph **I** of 4-methylhippuric acid: (a) front view and (b) back view in d_{norm}, (c) front view and (d) back view in *shape index*.

(a)



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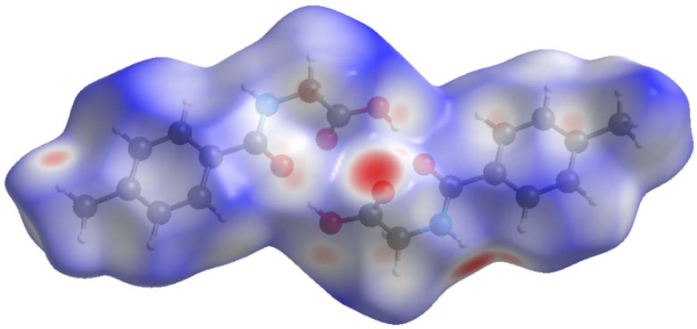

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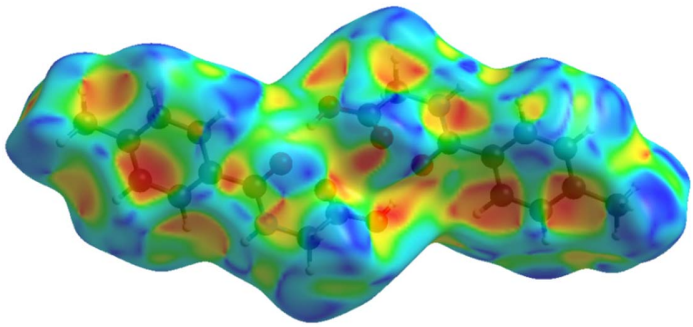


(d)

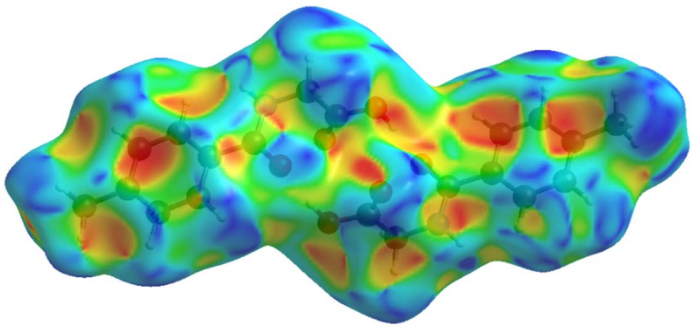
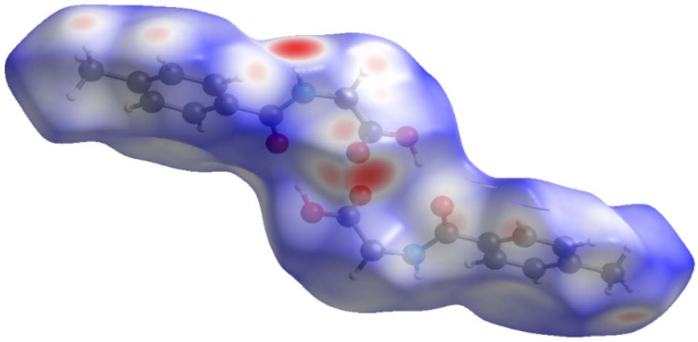


Figure S3 Views of Hirshfeld surface for dimer AA of polymorph **II** to 4-methylhippuric acid: (a) front view and (b) back view in d_{norm}, (c) front view and (d) back view in *shape index*.

(a)



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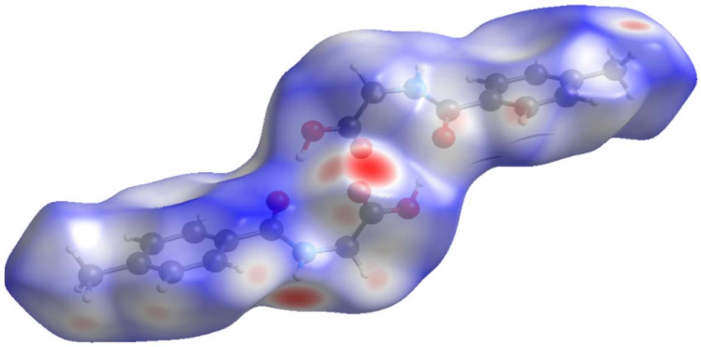
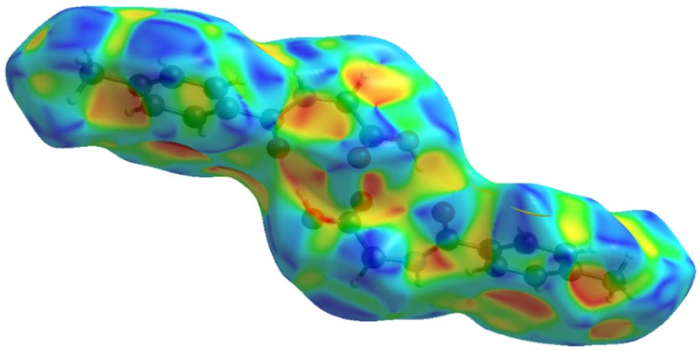


(c)



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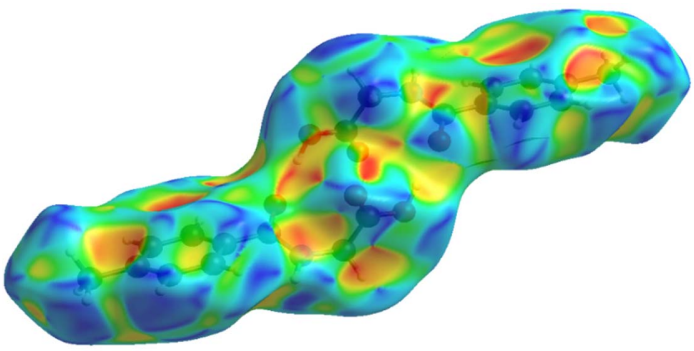

Figure S4 Views of Hirshfeld surface for dimer BB of polymorph **II** to 4-methylhippuric acid: (a) front view and (b) back view in d_{norm}, (c) front view and (d) back view in *shape index*.