

Topological electron density analysis and the electrostatic properties of isoniazid: An experimental and theoretical study

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Contents:

1. Table S1. Geometric parameters of isoniazid molecule
2. Figure S1. Residual map of isoniazid

Table S1. Geometric parameters of isoniazid molecule.

Bond lengths (Å)

C(1)–C(2)	1.3930(2)
C(1)–C(5)	1.3902(5)
C(2)–C(3)	1.3968(2)
C(2)–C(6)	1.5012(2)
C(3)–C(4)	1.3922(3)
C(4)–N(1)	1.3416(3)
C(5)–N(1)	1.3411(3)
C(6)–N(2)	1.3469(2)
N(2)–N(3)	1.4161(4)
C(6)–O(1)	1.2319(2)
C(1)–H(1)	1.0830(2)
C(3)–H(3)	1.0830(2)
C(4)–H(4)	1.0830(2)
C(5)–H(5)	1.0830(2)
N(2)–H(2)	1.0990(2)
N(3)–H(3A)	1.0090(2)
N(3)–H(3B)	1.0990(2)

Bond angles (°)

C(1)–C(2)–C(3)	118.27(2)
C(1)–C(2)–C(6)	118.25(2)
C(2)–C(1)–C(5)	118.84(2)
C(2)–C(3)–C(4)	118.71(2)
C(3)–C(2)–C(6)	123.46(2)
C(4)–N(1)–C(5)	117.49(2)
N(1)–C(4)–C(3)	123.30(2)
N(1)–C(5)–C(1)	123.38(2)
N(2)–C(6)–C(2)	115.79(1)
O(1)–C(6)–C(2)	121.74(2)
O(1)–C(6)–N(2)	122.46(2)
C(1)–C(5)–H(5)	121.58(2)
C(2)–C(1)–H(1)	123.71(2)
C(2)–C(3)–H(3)	124.37(2)
C(3)–C(4)–H(4)	119.58(2)

C(4)–C(3)–H(3)	116.75(2)
C(5)–C(1)–H(1)	117.45(2)
C(6)–N(2)–H(2)	123.35(2)
N(1)–C(4)–H(4)	117.11(2)
N(1)–C(5)–H(5)	115.03(2)
H(2)–N(2)–N(3)	116.45(2)
H(3A)–N(3)–H(3B)	108.94(1)
H(3A)–N(3)–N(2)	107.12(2)
H(3B)–N(3)–N(2)	107.80(3)

Torsion angles (°)

C(1)–C(2)–C(3)–C(4)	-0.5(1)
C(1)–C(2)–C(6)–N(2)	163.2(1)
C(1)–C(2)–C(6)–O(1)	-18.1(1)
C(2)–C(1)–C(5)–N(1)	-0.7(1)
C(2)–C(3)–C(4)–N(1)	0.1(1)
C(3)–C(2)–C(6)–N(2)	-18.1(1)
C(3)–C(2)–C(6)–O(1)	160.6(1)
C(4)–N(1)–C(5)–C(1)	0.3(1)
C(5)–C(1)–C(2)–C(3)	0.7(1)
C(5)–C(1)–C(2)–C(6)	179.5(1)
C(5)–N(1)–C(4)–C(3)	0.0(1)
C(6)–C(2)–C(3)–C(4)	-179.2(1)
C(1)–C(2)–C(3)–H(3)	174.9(1)
C(2)–C(1)–C(5)–H(5)	178.2(1)
C(2)–C(3)–C(4)–H(4)	179.1(1)
C(4)–N(1)–C(5)–H(5)	-178.8(1)
C(5)–N(1)–C(4)–H(4)	-179.0(1)
C(6)–C(2)–C(3)–H(3)	-3.9(1)
N(3)–N(2)–C(6)–C(2)	-173.0(2)
N(3)–N(2)–C(6)–O(1)	5.7(1)
H(1)–C(1)–C(2)–C(3)	-178.7(1)
H(1)–C(1)–C(2)–C(6)	0.1(1)
H(1)–C(1)–C(5)–H(5)	-2.2(1)
H(1)–C(1)–C(5)–N(1)	178.8(1)
H(2)–N(2)–C(6)–C(2)	-5.3(1)
H(2)–N(2)–C(6)–O(1)	176.0(1)
H(3)–C(3)–C(4)–H(4)	3.4(1)
H(3)–C(3)–C(4)–N(1)	-175.6(1)
H(3A)–N(3)–N(2)–C(6)	27(1)
H(3A)–N(3)–N(2)–H(2)	-150.5(1)

H(3B)–N(3)– N(2)–C(6)	-88.5(1)
H(3B)–N(3)– N(2)–H(2)	94.0(1)

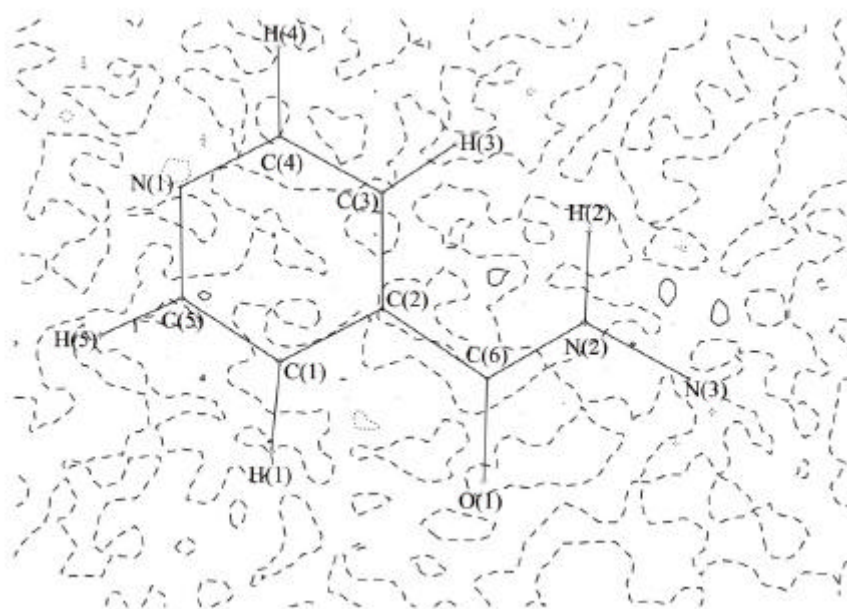


Figure S1. Residual map of isoniazid, solid lines show the positive contours and dotted lines represents negative contours and dashed lines are zero contours. The contours are drawn at 0.05 e^Å⁻³.