TABLE S1. DFT(B3LYP)/6-311++G(d,p) and MP2/6-31++G(d,p) optimized structural parameters and experimental geometries for the tree conformers of isoniazid.[a]

Parameter	Theoretical						Exp *(37)*	Parameter	Theoretical						Exp *(37)*
	C1		C2		T				C1		C2		T		
	DFT	MP2	DFT	MP2	DFT	MP2	X-ray diffraction		DFT	MP2	DFT	MP2	DFT	MP2	X-ray diffraction
Bond length / pm								**Bond length / pm**							
N_1-C_2	133.5	134.7	133.5	134.7	133.6	134.8	133.5	C_5-H_9	108.3	108.2	108.3	108.2	108.3	108.3	103.5
N_1-C_6	133.8	134.9	133.8	134.9	133.7	134.8	133.4	C_6-H_{10}	108.6	108.4	108.6	108.4	108.6	108.4	100.7
C_2-C_3	139.4	139.7	139.4	139.8	139.3	139.6	139.4	C_{11}=O_{12}	122.1	123.7	121.3	122.9	122.1	123.6	123.4
C_2-H_7	108.6	108.4	108.6	108.4	108.6	108.4	103.3	C_{11}-N_{13}	137.1	137.2	137.8	138.0	137.7	138.0	133.2
C_3-C_4	139.7	140.0	139.7	140.0	139.6	139.9	138.8	N_{13}-N_{14}	140.8	141.1	139.7	140.2	140.3	140.9	141.3
C_3-H_8	108.6	108.3	108.4	108.3	108.0	108.1	103.9	N_{13}-H_{15}	100.9	101.0	101.2	101.3	101.5	101.6	110.0
C_4-C_5	139.5	139.9	139.5	139.9	139.6	140.0	140.3	N_{14}-H_{16}	101.9	101.9	101.4	101.4	101.4	101.4	107.0
C_4-C_{11}	150.5	149.5	151.1	150.1	150.4	149.4	148.5	N_{14}-H_{17}	101.7	101.6	101.3	101.2	101.6	101.6	102.0
C_5-C_6	139.2	139.5	139.2	139.5	139.2	139.6	138.5								
Bond angles / °								**Bond angles / °**							
C_2-N_1-C_6	117.2	116.8	117.2	116.7	117.1	116.7	116.5	N_1-C_6-C_5	123.7	123.9	123.7	123.9	123.6	123.8	124.1
N_1-C_2-C_3	123.7	123.9	123.7	123.9	123.9	124.0	123.6	N_1-C_6-H_{10}	116.1	115.7	116.1	115.7	116.2	115.8	114.3
N_1-C_2-H_7	116.2	115.8	116.2	115.8	116.1	115.7	115.3	C_5-C_6-H_{10}	120.2	120.5	120.2	120.5	120.2	120.4	121.2
C_3-C_2-H_7	120.1	120.3	120.1	120.4	120.0	120.3	121.0	C_4-C_{11}=O_{12}	122.3	122.8	121.6	122.2	120.9	121.6	122.2
C_2-C_3-C_4	118.7	118.5	118.8	118.6	118.6	118.4	119.8	C_4-C_{11}-N_{13}	115.7	114.7	113.8	112.8	119.7	117.9	115.5
C_2-C_3-H_8	119.6	120.2	119.5	120.1	120.0	120.4	122.8	N_{13}-C_{11}=O_{12}	122.1	122.5	124.5	125.0	119.4	120.4	122.0
C_4-C_3-H_8	121.7	121.3	121.7	121.3	121.4	121.2	117.6	C_{11}-N_{13}-N_{14}	121.2	120.5	120.5	119.2	123.8	120.6	120.7
C_3-C_4-C_5	118.0	118.5	117.8	118.3	117.9	118.4	116.5	C_{11}-N_{13}-H_{15}	119.7	119.0	118.3	117.0	113.0	112.7	128.0
C_3-C_4-C_{11}	123.6	122.7	124.0	123.1	124.7	123.4	125.2	N_{14}-N_{13}-H_{15}	114.2	114.0	119.5	119.2	119.5	119.0	112.0
C_5-C_4-C_{11}	118.3	118.8	118.1	118.6	117.3	118.0	118.3	N_{13}-N_{14}-H_{16}	107.8	107.4	111.5	111.1	109.9	108.9	107.8
C_4-C_5-C_6	118.7	118.6	118.8	118.7	118.9	118.7	119.4	N_{13}-N_{14}-H_{17}	108.2	107.5	110.4	109.2	111.0	110.5	109.8
C_4-C_5-H_9	119.9	120.1	119.8	120.0	120.0	120.2	118.0	H_{16}-N_{14}-H_{17}	106.4	106.3	110.7	110.4	109.4	109.2	111.9
C_6-C_5-H_9	121.4	121.3	121.3	121.3	121.0	121.1	122.9								
Dihedral angles / °															
C_6-N_1-C_2-C_3	0.7	0.5	0.9	0.7	1.1	0.9	1.4	C_3-C_4-C_{11}=O_{12}	153.9	144.6	149.0	141.2	143.2	136.0	160.8
C_6-N_1-C_2-H_7	-179.9	-179.0	-178.8	-178.8	-179.2	-179.2	-175.9	C_3-C_4-C_{11}-N_{13}	-26.1	-34.8	-31.2	-38.3	-35.4	-41.2	-17.1
C_2-N_1-C_6-C_5	-0.2	-0.5	-0.2	-0.5	0.2	-0.01	-1.2	C_5-C_4-C_{11}=O_{12}	-24.6	-33.8	-28.9	-36.6	-32.1	-38.9	-18.2
C_2-N_1-C_6-H_{10}	179.7	179.6	179.6	179.5	179.7	179.6	177.4	C_5-C_4-C_{11}-N_{13}	155.3	146.7	151.0	143.9	149.2	143.8	163.9
N_1-C_2-C_3-C_4	-0.3	0.3	-0.4	-0.1	-1.1	-0.6	-1.0	C_4-C_5-C_6-N_1	-0.8	-0.3	-0.9	-0.6	-1.4	-1.2	-0.7
N_1-C_2-C_3-H_8	-178.2	-178.0	-178.2	-178.0	179.2	179.8	-169.7	C_4-C_5-C_6-H_{10}	179.4	179.6	179.3	179.5	179.1	179.2	177.8
H_7-C_2-C_3-C_4	179.4	179.7	179.2	179.6	179.2	179.5	176.1	H_9-C_5-C_6-N_1	179.0	179.2	178.6	178.9	178.0	178.2	170.5
H_7-C_2-C_3-H_8	1.4	1.4	1.5	1.5	-0.5	-0.2	13.2	H_9-C_5-C_6-H_{10}	-0.8	-0.9	-1.1	-1.1	-1.5	-1.4	-11.0
C_2-C_3-C_4-C_5	-0.7	-1.1	-0.7	-1.1	-0.2	-0.6	-0.5	C_4-C_{11}-N_{13}-N_{14}	-174.0	-173.3	-179.2	-177.2	-18.3	-25.1	-173.0
C_2-C_3-C_4-C_{11}	-179.2	-179.6	-178.6	-178.9	-175.5	-175.6	-179.4	C_4-C_{11}-N_{13}-H_{15}	-20.2	-23.7	-14.5	-21.5	-176.5	-174.4	-0.6
H_8-C_3-C_4-C_5	177.3	177.2	177.0	177.0	179.5	179.0	170.7	O_{12}=C_{11}-N_{13}-N_{14}	6.0	7.2	0.7	3.3	163.1	157.6	4.9
H_8-C_3-C_4-C_{11}	-1.3	-1.3	-0.9	-0.8	4.2	4.1	-8.3	O_{12}=C_{11}-N_{13}-H_{15}	159.8	156.9	165.3	159.0	4.8	8.4	178.5
C_3-C_4-C_5-C_6	1.1	1.1	1.3	1.3	1.3	1.5	0.3	C_{11}-N_{13}-N_{14}-H_{16}	32.4	32.4	105.7	100.3	136.7	141.0	30.1
C_3-C_4-C_5-H_9	-178.6	-178.4	-178.3	-178.1	-178.0	-177.9	-171.3	C_{11}-N_{13}-N_{14}-H_{17}	-82.2	-81.7	-130.5	-137.8	-102.1	-99.1	-92.1
C_{11}-C_4-C_5-C_6	179.8	179.7	179.3	179.2	177.0	176.7	179.4	H_{15}-N_{13}-N_{14}-H_{16}	-122.6	-118.7	-58.8	-54.8	-66.3	-71.7	-144.4
C_{11}-C_4-C_5-H_9	0.02	0.2	-0.3	-0.3	-2.4	-2.7	7.7	H_{15}-N_{13}-N_{14}-H_{17}	122.7	127.2	64.7	67.1	54.8	48.2	93.4

[a] See Scheme 1 for atom numbering.