Supplemental Materials

The atomic numbering used in the Z-matrix formulation is shown in Figs. 1 and 2. Tables showing the refined values for all structural parameters, compared to those refined from the data set free of impurity, are included for comparison between refinement methods. The fractional coordinates of the molecules, x, y, and z, give the geometric center of the aromatic rings. All parameters were allowed to refine free from any constraints. The refined structures and data for the acetaminophen and ibuprofen mixtures are included in CIF format, and may be obtained online.

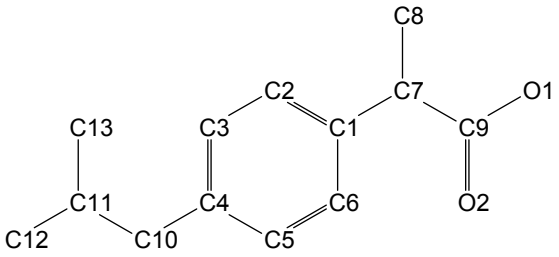

Fig. 1. Schematic of the ibuprofen molecule as modeled using Z-matrices showing the numbering of the non-Hydrogen atoms.

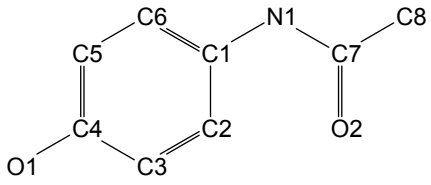

Fig. 2. Schematic of the acetaminophen molecule as modeled using Z-matrices showing the numbering of the non-Hydrogen atoms.

Table 1. *A comparison of the refined structural parameters for ibuprofen between the data taken on a pure sample, and one composed of only 68% ibuprofen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Ibuprofen			**68% Ibuprofen**		
	McConnell (1974)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	14.667	14.6696(7)	14.6712(7)	14.6662(9)	14.6690(9)	14.6682(8)
b(Å)	7.886	7.8890(3)	7.8893(3)	7.8879(4)	7.8884(3)	7.8889(4)
c(Å)	10.73	10.7287(3)	10.7288(3)	10.7275(4)	10.7281(4)	10.7276(4)
β(°)	99.362	99.427(2)	99.428(2)	99.432(3)	99.429(3)	99.437(3)
B (isotropic)		4.2(2)	4.3(2)	4.5(3)	4.6(3)	4.6(3)
aromatic(Å)	1.383	1.402(3)	1.400(3)	1.394(4)	1.413(4)	1.400(4)
C-C bond (Å)	1.518	1.557(6)	1.560(5)	1.60(1)	1.565(9)	1.610(8)
O1-C9 bond (Å)	1.305	1.28(2)	1.26(2)	1.27(3)	1.32(3)	1.27(3)
O2-C9 bond (Å)	1.221	1.16(2)	1.26(2)	1.08(3)	1.16(3)	1.14(3)
x		0.7403(3)	0.7395(3)	0.7398(4)	0.7397(4)	0.7402(4)
y		-0.4571(5)	0.5420(5)	0.5406(9)	-0.4578(8)	0.5421(8)
z		0.9847(6)	0.9836(5)	0.9855(9)	0.9844(8)	0.9852(7)
Rotation around x (°)		12.1(3)	13.0(3)	10.9(5)	10.6(5)	11.6(5)
Rotation around y (°)		137.3(1)	136.6(1)	137.1(2)	137.3(2)	136.8(2)
Rotation around z (°)		-222.7(3)	-222.2(2)	-223.7(4)	-223.2(4)	-223.3(3)
C8-C7-C1 angle (°)	114.35	111.4(6)	111.9(6)	109(1)	112(1)	106.6(9)
C9-C7-C1 angle (°)	107.17	111(1)	108.2(9)	109(2)	109(2)	107(1)
O1-C9-C7 angle (°)	114.53	257(1)	252(1)	260(2)	259(2)	260(2)
O2-C9-C7 angle (°)	122.9	128(2)	124(1)	128(3)	131(3)	127(2)
C11-C10-C4 angle (°)	113.62	112.5(8)	110.9(7)	108(1)	111(1)	107(1)
C12-C11-C10 angle (°)	110.58	104(1)	106(1)	10(2)	102(2)	99(1)
C13-C11-C10 angle (°)	111.98	107(1)	111(1)	103(2)	108(2)	105(2)
C8-C7-C1-C2 torsion (°)	42.05	35.3(9)	32.8(8)	34(1)	35(1)	33(1)
C9-C7-C1-C2 torsion (°)	-80.64	-77(1)	-80.8(9)	-76(1)	-76(1)	-77(1)
O1-C9-C7-C1 torsion (°)	-88.68	-91(2)	-90(2)	-94(3)	-91(2)	-96(2)
O2-C9-C7-C1 torsion (°)	89.28	76(3)	84(2)	76(5)	79(4)	82(4)
C11-C10-C4-C2 torsion (°)	-102.11	-102.8(8)	-102.4(7)	-108(1)	-105(1)	-106(1)
C12-C11-C10-C4 torsion (°)	-168.75	-164.5(7)	-165.4(7)	-169(1)	-165(1)	-168(1)
C13-C11-C10-C4 torsion (°)	67.29	69(1)	68(1)	75(2)	72(2)	74(2)

Table 2. *A comparison of the refined structural parameters for ibuprofen between the data taken on a pure sample, and one composed of only 56% ibuprofen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Ibuprofen			**55% Ibuprofen**		
	McConnell (1974)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	14.667	14.6696(7)	14.6712(7)	14.664(2)	14.6703(6)	14.6698(8)
b(Å)	7.886	7.8890(3)	7.8893(3)	7.8871(7)	7.8890(3)	7.8878(3)
c(Å)	10.73	10.7287(3)	10.7288(3)	10.7244(9)	10.7282(3)	10.7265(4)
β(°)	99.362	99.427(2)	99.428(2)	99.417(6)	99.429(2)	99.432(3)
B (isotropic)		4.2(2)	4.3(2)	3.5(5)	4.0(2)	3.0(2)
aromatic(Å)	1.383	1.402(3)	1.400(3)	1.37(1)	1.396(4)	1.409(4)
C-C bond (Å)	1.518	1.557(6)	1.560(5)	1.64(2)	1.545(6)	1.555(7)
O1-C9 bond (Å)	1.305	1.28(2)	1.26(2)	1.43(7)	1.30(2)	1.31(2)
O2-C9 bond (Å)	1.221	1.16(2)	1.26(2)	1.08(6)	1.15(2)	1.10(2)
x		0.7403(3)	0.7395(3)	0.7381(9)	0.7390(3)	0.7383(4)
y		-0.4571(5)	0.5420(5)	-0.456(2)	-0.4563(6)	-0.4556(7)
z		0.9847(6)	0.9836(5)	0.991(2)	0.9856(7)	0.9882(7)
Rotation around x (°)		12.1(3)	13.0(3)	12(1)	13.0(4)	13.9(4)
Rotation around y (°)		137.3(1)	136.6(1)	137.8(4)	137.7(2)	137.3(2)
Rotation around z (°)		-222.7(3)	-222.2(2)	-223.3(7)	-222.5(3)	-221.1(3)
C8-C7-C1 angle (°)	114.35	111.4(6)	111.9(6)	102(2)	112.0(7)	109.4(9)
C9-C7-C1 angle (°)	107.17	111(1)	108.2(9)	119(3)	114(1)	111(1)
O1-C9-C7 angle (°)	114.53	257(1)	252(1)	263(4)	256(2)	249(2)
O2-C9-C7 angle (°)	122.9	128(2)	124(1)	111(4)	126(2)	116(2)
C11-C10-C4 angle (°)	113.62	112.5(8)	110.9(7)	107(2)	114.4(9)	112.5(9)
C12-C11-C10 angle (°)	110.58	104(1)	106(1)	93(3)	108(1)	104(1)
C13-C11-C10 angle (°)	111.98	107(1)	111(1)	94(3)	106(1)	107(1)
C8-C7-C1-C2 torsion (°)	42.05	35.3(9)	32.8(8)	39(2)	40(1)	41(1)
C9-C7-C1-C2 torsion (°)	-80.64	-77(1)	-80.8(9)	-77(3)	-77(1)	-83(1)
O1-C9-C7-C1 torsion (°)	-88.68	-91(2)	-90(2)	-70(5)	-83(2)	-80(2)
O2-C9-C7-C1 torsion (°)	89.28	76(3)	84(2)	47(8)	68(3)	80(3)
C11-C10-C4-C2 torsion (°)	-102.11	-102.8(8)	-102.4(7)	-114(2)	-104(1)	-104(1)
C12-C11-C10-C4 torsion (°)	-168.75	-164.5(7)	-165.4(7)	-181(2)	-165.0(9)	-173.2(9)
C13-C11-C10-C4 torsion (°)	67.29	69(1)	68(1)	79(3)	66(2)	67(2)

Table 3. *A comparison of the refined structural parameters for ibuprofen between the data taken on a pure sample, and one composed of only 28% ibuprofen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Ibuprofen			**26% Ibuprofen**		
	McConnell (1974)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	14.667	14.6696(7)	14.6712(7)	14.499(3)	14.6706(9)	14.666(2)
b(Å)	7.886	7.8890(3)	7.8893(3)	7.758(1)	7.8885(4)	7.8817(8)
c(Å)	10.73	10.7287(3)	10.7288(3)	10.620(2)	10.7284(5)	10.7240(9)
β(°)	99.362	99.427(2)	99.428(2)	99.74(1)	99.426(4)	99.427(6)
B (isotropic)		4.2(2)	4.3(2)	20(1)	3.1(4)	0.3(4)
aromatic(Å)	1.383	1.402(3)	1.400(3)	2.81(3)	1.395(6)	1.435(7)
C-C bond (Å)	1.518	1.557(6)	1.560(5)	2.78(3)	1.54(1)	1.58(1)
O1-C9 bond (Å)	1.305	1.28(2)	1.26(2)	5.85(7)	1.38(4)	1.42(4)
O2-C9 bond (Å)	1.221	1.16(2)	1.26(2)	4.51(7)	1.20(4)	1.62(5)
x		0.7403(3)	0.7395(3)	0.7469(9)	0.7391(5)	0.7350(6)
y		-0.4571(5)	0.5420(5)	-0.405(3)	-0.459(1)	-0.492(1)
z		0.9847(6)	0.9836(5)	0.841(3)	0.980(1)	0.968(1)
Rotation around x (°)		12.1(3)	13.0(3)	-22.3(7)	11.4(7)	14.6(7)
Rotation around y (°)		137.3(1)	136.6(1)	128.8(5)	138.1(3)	141.6(3)
Rotation around z (°)		-222.7(3)	-222.2(2)	-251.3(5)	-223.6(5)	-219.7(6)
C8-C7-C1 angle (°)	114.35	111.4(6)	111.9(6)	47(1)	113(1)	104(2)
C9-C7-C1 angle (°)	107.17	111(1)	108.2(9)	129(2)	121(2)	137(2)
O1-C9-C7 angle (°)	114.53	257(1)	252(1)	336(1)	266(3)	243(3)
O2-C9-C7 angle (°)	122.9	128(2)	124(1)	60(1)	129(4)	78(2)
C11-C10-C4 angle (°)	113.62	112.5(8)	110.9(7)	79(1)	114(2)	106(2)
C12-C11-C10 angle (°)	110.58	104(1)	106(1)	94(2)	111(2)	78(2)
C13-C11-C10 angle (°)	111.98	107(1)	111(1)	142(2)	105(2)	90(2)
C8-C7-C1-C2 torsion (°)	42.05	35.3(9)	32.8(8)	42(2)	39(2)	64(2)
C9-C7-C1-C2 torsion (°)	-80.64	-77(1)	-80.8(9)	-313(2)	-70(3)	-134(4)
O1-C9-C7-C1 torsion (°)	-88.68	-91(2)	-90(2)	93(3)	-84(3)	-161(6)
O2-C9-C7-C1 torsion (°)	89.28	76(3)	84(2)	274(2)	42(7)	99(3)
C11-C10-C4-C2 torsion (°)	-102.11	-102.8(8)	-102.4(7)	-125(2)	-104(2)	-117(2)
C12-C11-C10-C4 torsion (°)	-168.75	-164.5(7)	-165.4(7)	-320(1)	65(3)	-177(2)
C13-C11-C10-C4 torsion (°)	67.29	69(1)	68(1)	20(4)	-161(2)	69(2)

Table 4. *A comparison of the refined structural parameters for ibuprofen between the data taken on a pure sample, and one composed of only 19% ibuprofen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Ibuprofen			**17% Ibuprofen**		
	McConnell (1974)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	14.667	14.6696(7)	14.6712(7)	14.494(3)	14.673(1)	14.669(2)
b(Å)	7.886	7.8890(3)	7.8893(3)	7.753(1)	7.8892(6)	7.880(1)
c(Å)	10.73	10.7287(3)	10.7288(3)	10.666(2)	10.7316(6)	10.727(1)
β(°)	99.362	99.427(2)	99.428(2)	99.88(1)	99.436(5)	99.439(8)
B (isotropic)		4.2(2)	4.3(2)	20(2)	3.4(6)	-1.3(4)
aromatic(Å)	1.383	1.402(3)	1.400(3)	2.4(3)	1.400(8)	1.59(1)
C-C bond (Å)	1.518	1.557(6)	1.560(5)	3.65(3)	1.56(2)	1.70(1)
O1-C9 bond (Å)	1.305	1.28(2)	1.26(2)	5.14(7)	1.46(6)	2.06(5)
O2-C9 bond (Å)	1.221	1.16(2)	1.26(2)	2.09(6)	1.22(6)	2.29(5)
x		0.7403(3)	0.7395(3)	0.758(1)	0.7391(8)	0.7375(7)
y		-0.4571(5)	0.5420(5)	-0.416(3)	-0.459(2)	-0.482(2)
z		0.9847(6)	0.9836(5)	0.942(3)	0.981(2)	0.971(1)
Rotation around x (°)		12.1(3)	13.0(3)	-6.3(8)	12(1)	1.5(7)
Rotation around y (°)		137.3(1)	136.6(1)	128.3(4)	138.9(4)	144.8(3)
Rotation around z (°)		-222.7(3)	-222.2(2)	-230.7(6)	-224.0(8)	-223.3(5)
C8-C7-C1 angle (°)	114.35	111.4(6)	111.9(6)	28(1)	107(2)	80(2)
C9-C7-C1 angle (°)	107.17	111(1)	108.2(9)	87(1)	127(3)	131(2)
O1-C9-C7 angle (°)	114.53	257(1)	252(1)	317(1)	271(4)	282(2)
O2-C9-C7 angle (°)	122.9	128(2)	124(1)	64(1)	119(5)	48(2)
C11-C10-C4 angle (°)	113.62	112.5(8)	110.9(7)	45(1)	114(2)	112(2)
C12-C11-C10 angle (°)	110.58	104(1)	106(1)	77.9(9)	106(3)	71(2)
C13-C11-C10 angle (°)	111.98	107(1)	111(1)	153(2)	103(3)	74(2)
C8-C7-C1-C2 torsion (°)	42.05	35.3(9)	32.8(8)	12(2)	42(3)	48(2)
C9-C7-C1-C2 torsion (°)	-80.64	-77(1)	-80.8(9)	-48(2)	-66(4)	-177(3)
O1-C9-C7-C1 torsion (°)	-88.68	-91(2)	-90(2)	-48(1)	-82(4)	-105(2)
O2-C9-C7-C1 torsion (°)	89.28	76(3)	84(2)	-31(3)	28(8)	131(2)
C11-C10-C4-C2 torsion (°)	-102.11	-102.8(8)	-102.4(7)	-96(1)	-106(2)	-102(2)
C12-C11-C10-C4 torsion (°)	-168.75	-164.5(7)	-165.4(7)	-120(2)	66(4)	-182(2)
C13-C11-C10-C4 torsion (°)	67.29	69(1)	68(1)	-3(4)	-159(2)	38(2)

Table 5. *A comparison of the refined structural parameters for ibuprofen between the data taken on a pure sample, and one composed of only 6% ibuprofen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Ibuprofen			**5% Ibuprofen**		
	McConnell (1974)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	14.667	14.6696(7)	14.6712(7)	14.528(4)	14.670(2)	14.683(4)
b(Å)	7.886	7.8890(3)	7.8893(3)	7.77(2)	7.889(1)	7.860(2)
c(Å)	10.73	10.7287(3)	10.7288(3)	10.691(3)	10.730(1)	10.729(2)
β(°)	99.362	99.427(2)	99.428(2)	99.89(2)	99.43(1)	99.46(2)
B (isotropic)		4.2(2)	4.3(2)	20(2)	-0.6(8)	-6.7(4)
aromatic(Å)	1.383	1.402(3)	1.400(3)	2.24(2)	1.44(2)	1.70(2)
C-C bond (Å)	1.518	1.557(6)	1.560(5)	3.07(4)	1.63(3)	177(2)
O1-C9 bond (Å)	1.305	1.28(2)	1.26(2)	3.7(1)	1.7(1)	1.49(7)
O2-C9 bond (Å)	1.221	1.16(2)	1.26(2)	3.5(2)	1.4(1)	1.14(6)
x		0.7403(3)	0.7395(3)	0.769(1)	0.736(1)	0.757(1)
y		-0.4571(5)	0.5420(5)	-0.435(3)	-0.486(4)	-0.439(2)
z		0.9847(6)	0.9836(5)	0.969(2)	0.970(3)	1.027(2)
Rotation around x (°)		12.1(3)	13.0(3)	20(1)	9(2)	14.9(9)
Rotation around y (°)		137.3(1)	136.6(1)	150.5(4)	141.2(7)	139.1(4)
Rotation around z (°)		-222.7(3)	-222.2(2)	-217.9(6)	-227(1)	-222.4(5)
C8-C7-C1 angle (°)	114.35	111.4(6)	111.9(6)	33(2)	101(3)	50(2)
C9-C7-C1 angle (°)	107.17	111(1)	108.2(9)	72(3)	146(5)	110(2)
O1-C9-C7 angle (°)	114.53	257(1)	252(1)	304(2)	280(5)	271(3)
O2-C9-C7 angle (°)	122.9	128(2)	124(1)	39(2)	105(6)	92(3)
C11-C10-C4 angle (°)	113.62	112.5(8)	110.9(7)	34(2)	109(4)	135(2)
C12-C11-C10 angle (°)	110.58	104(1)	106(1)	69(2)	80(4)	75(3)
C13-C11-C10 angle (°)	111.98	107(1)	111(1)	139(3)	91(5)	57(2)
C8-C7-C1-C2 torsion (°)	42.05	35.3(9)	32.8(8)	32(3)	48(4)	61(3)
C9-C7-C1-C2 torsion (°)	-80.64	-77(1)	-80.8(9)	-80(3)	-57(9)	-71(2)
O1-C9-C7-C1 torsion (°)	-88.68	-91(2)	-90(2)	-63(2)	-83(9)	-51(4)
O2-C9-C7-C1 torsion (°)	89.28	76(3)	84(2)	155(2)	0(1)	62(4)
C11-C10-C4-C2 torsion (°)	-102.11	-102.8(8)	-102.4(7)	-76(2)	-125(3)	-83(3)
C12-C11-C10-C4 torsion (°)	-168.75	-164.5(7)	-165.4(7)	-236(3)	72(4)	-192(2)
C13-C11-C10-C4 torsion (°)	67.29	69(1)	68(1)	-82(4)	-156(4)	11(3)

Table 6. *A comparison of the refined structural parameters for acetaminophen between the data taken on a pure sample, and one composed of only 93% acetaminophen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Acetaminophen			**93% Acetaminophen**		
	Haisa (1976)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	12.93	12.8861(2)	12.8856(2)	12.8865(2)	12.8900(2)	12.8863(2)
b(Å)	9.40	9.3812(1)	9.3801(1)	9.3822(2)	9.3847(1)	9.3816(2)
c(Å)	7.10	7.1010(1)	7.1010(1)	7.1015(1)	7.1033(1)	7.1016(1)
β(°)	115.9	115.7015(8)	115.7002(9)	115.702(1)	115.7017(9)	115.701(1)
B (isotropic)		3.14(7)	2.76(7)	3.4(1)	3.30(8)	2.89(8)
aromatic(Å)	1.388	1.387(2)	1.382(2)	1.390(2)	1.389(2)	1.387(2)
N1-C1 bond (Å)	1.425	1.406(4)	1.411(4)	1.386(6)	1.391(5)	1.400(5)
C7-N1 bond (Å)	1.341	1.337(7)	1.325(7)	1.33(1)	1.345(8)	1.333(8)
O2-C7 bond (Å)	1.232	1.244(7)	1.237(7)	1.246(1)	1.230(8)	1.224(8)
C8-C7 bond (Å)	1.509	1.507(7)	1.505(6)	1.539(9)	1.512(7)	1.516(8)
O1-C4 bond (Å)	1.377	1.391(4)	1.402(4)	1.391(6)	1.396(5)	1.399(5)
x		16.5347(2)	16.5345(2)	16.5338(4)	16.5347(3)	16.5342(3)
y		8.2627(3)	8.2629(2)	8.2625(4)	8.2628(3)	8.2630(3)
z		-0.0777(4)	-0.0784(3)	-0.0795(5)	-0.0776(4)	-0.0799(4)
Rotation around x (°)		-227.4(1)	-227.5(1)	-227.1(2)	-227.3(1)	-227.2(1)
Rotation around y (°)		199.3(2)	199.4(2)	199.4(2)	199.2(2)	199.6(2)
Rotation around z (°)		-219.3(2)	-219.4(2)	-219.4(3)	-219.3(2)	-219.6(2)
N1-C1-C2 angle (°)	124.3	121.4(5)	121.7(5)	123.0(8)	121.6(6)	123.4(6)
C7-N1-C1 angle (°)	128.2	132.4(7)	131.8(6)	129.4(9)	132.3(7)	129.2(8)
O2-C7-N1 angle (°)	122.8	121.4(7)	122.0(6)	124.5(9)	121.4(7)	123.4(8)
C8-C7-N1 angle (°)	114.69	119.3(5)	119.1(5)	119.5(7)	119.2(6)	118.8(6)
O1-C4-C5 angle (°)	117.7	120.4(5)	120.6(4)	120.1(7)	119.7(6)	120.6(5)
N1-C1-C2-C3 torsion (°)	179.8	179.3(5)	178.9(4)	178.2(7)	179.4(5)	178.0(5)
C7-N1-C1-C2 torsion (°)	23.4	20.4(9)	21.7(8)	22(1)	20(1)	23(1)
O2-C7-N1-C1 torsion (°)	-2.2	3(1)	1(1)	2(2)	4(1)	0(1)
C8-C7-N1-C1 torsion (°)	177.68	177.4(6)	177.8(5)	176.2(8)	176.5(7)	176.3(6)
O1-C4-C5-C6 torsion (°)	-178.8	-175.7(4)	-175.9(4)	-175.8(6)	-175.7(5)	-176.0(5)

Table 7. *A comparison of the refined structural parameters for acetaminophen between the data taken on a pure sample, and one composed of only 79% acetaminophen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Acetaminophen			**80% Acetaminophen**		
	Haisa (1976)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	12.93	12.8861(2)	12.8856(2)	12.8871(4)	12.8905(2)	12.8870(3)
b(Å)	9.40	9.3812(1)	9.3801(1)	9.3824(3)	9.3849(2)	9.3819(2)
c(Å)	7.10	7.1010(1)	7.1010(1)	7.1018(3)	7.1034(1)	7.1015(2)
β(°)	115.9	115.7015(8)	115.7002(9)	115.703(2)	115.701(1)	115.701(1)
B (isotropic)		3.14(7)	2.76(7)	3.6(2)	3.4(1)	3.1(1)
aromatic(Å)	1.388	1.387(2)	1.382(2)	1.392(4)	1.381(3)	1.393(2)
N1-C1 bond (Å)	1.425	1.406(4)	1.411(4)	1.38(1)	1.37(1)	1.396(7)
C7-N1 bond (Å)	1.341	1.337(7)	1.325(7)	1.35(2)	1.368(9)	1.34(1)
O2-C7 bond (Å)	1.232	1.244(7)	1.237(7)	1.23(2)	1.22(1)	1.21(1)
C8-C7 bond (Å)	1.509	1.507(7)	1.505(6)	1.56(2)	1.501(9)	1.53(1)
O1-C4 bond (Å)	1.377	1.391(4)	1.402(4)	1.40(1)	1.402(6)	1.400(7)
x		16.5347(2)	16.5345(2)	16.5327(7)	16.5344(4)	16.5336(4)
y		8.2627(3)	8.2629(2)	8.2625(7)	8.2625(4)	8.2625(4)
z		-0.0777(4)	-0.0784(3)	-0.0835(9)	-0.0775(6)	-0.0811(6)
Rotation around x (°)		-227.4(1)	-227.5(1)	-227.0(3)	-227.7(2)	-227.1(2)
Rotation around y (°)		199.3(2)	199.4(2)	200.0(5)	199.1(3)	199.7(3)
Rotation around z (°)		-219.3(2)	-219.4(2)	-219.8(5)	-219.2(3)	-219.8(3)
N1-C1-C2 angle (°)	124.3	121.4(5)	121.7(5)	126(1)	123.0(9)	124.0(9)
C7-N1-C1 angle (°)	128.2	132.4(7)	131.8(6)	124(2)	130.9(9)	127(1)
O2-C7-N1 angle (°)	122.8	121.4(7)	122.0(6)	128(2)	122.0(9)	126(1)
C8-C7-N1 angle (°)	114.69	119.3(5)	119.1(5)	119(1)	115.6(7)	117.3(8)
O1-C4-C5 angle (°)	117.7	120.4(5)	120.6(4)	121(1)	119.6(7)	121.3(8)
N1-C1-C2-C3 torsion (°)	179.8	179.3(5)	178.9(4)	176(1)	178.9(7)	177.3(8)
C7-N1-C1-C2 torsion (°)	23.4	20.4(9)	21.7(8)	24(2)	19(1)	24(1)
O2-C7-N1-C1 torsion (°)	-2.2	3(1)	1(1)	-2(3)	6(2)	-2(2)
C8-C7-N1-C1 torsion (°)	177.68	177.4(6)	177.8(5)	176(1)	175.8(8)	175.7(9)
O1-C4-C5-C6 torsion (°)	-178.8	-175.7(4)	-175.9(4)	-177(1)	-176.8(6)	-176.9(7)

Table 8. *A comparison of the refined structural parameters for acetaminophen between the data taken on a pure sample, and one composed of only 69% acetaminophen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Acetaminophen			**70% Acetaminophen**		
	Haisa (1976)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	12.93	12.8861(2)	12.8856(2)	12.8858(6)	12.8890(2)	12.8856(3)
b(Å)	9.40	9.3812(1)	9.3801(1)	9.3812(4)	9.3835(2)	9.3812(2)
c(Å)	7.10	7.1010(1)	7.1010(1)	7.1013(4)	7.1027(1)	7.1011(2)
β(°)	115.9	115.7015(8)	115.7002(9)	115.703(3)	115.702(1)	115.697(2)
B (isotropic)		3.14(7)	2.76(7)	3.7(3)	3.4(1)	3.2(1)
aromatic(Å)	1.388	1.387(2)	1.382(2)	1.393(6)	1.386(2)	1.395(3)
N1-C1 bond (Å)	1.425	1.406(4)	1.411(4)	1.37(2)	1.387(7)	1.404(8)
C7-N1 bond (Å)	1.341	1.337(7)	1.325(7)	1.35(3)	1.35(1)	1.33(1)
O2-C7 bond (Å)	1.232	1.244(7)	1.237(7)	1.24(2)	1.23(1)	1.19(1)
C8-C7 bond (Å)	1.509	1.507(7)	1.505(6)	1.58(2)	1.51(1)	1.54(1)
O1-C4 bond (Å)	1.377	1.391(4)	1.402(4)	1.40(2)	1.402(6)	1.401(7)
x		16.5347(2)	16.5345(2)	16.532(1)	16.5343(4)	16.5335(5)
y		8.2627(3)	8.2629(2)	8.262(1)	8.2625(4)	8.2625(5)
z		-0.0777(4)	-0.0784(3)	-0.086(1)	-0.0767(6)	-0.0824(6)
Rotation around x (°)		-227.4(1)	-227.5(1)	-226.9(4)	-227.9(2)	-227.1(2)
Rotation around y (°)		199.3(2)	199.4(2)	200.4(7)	199.1(3)	199.9(1)
Rotation around z (°)		-219.3(2)	-219.4(2)	-219.2(7)	-218.6(3)	-220.0(3)
N1-C1-C2 angle (°)	124.3	121.4(5)	121.7(5)	127(2)	119.7(9)	125(1)
C7-N1-C1 angle (°)	128.2	132.4(7)	131.8(6)	120(2)	133(1)	124(1)
O2-C7-N1 angle (°)	122.8	121.4(7)	122.0(6)	133(2)	122(1)	129(1)
C8-C7-N1 angle (°)	114.69	119.3(5)	119.1(5)	119(2)	117.1(8)	114.1(9)
O1-C4-C5 angle (°)	117.7	120.4(5)	120.6(4)	119(2)	119.0(8)	121.5(9)
N1-C1-C2-C3 torsion (°)	179.8	179.3(5)	178.9(4)	173(2)	178.4(7)	177.1(8)
C7-N1-C1-C2 torsion (°)	23.4	20.4(9)	21.7(8)	28(3)	18(1)	23(1)
O2-C7-N1-C1 torsion (°)	-2.2	3(1)	1(1)	-4(5)	11(2)	1(2)
C8-C7-N1-C1 torsion (°)	177.68	177.4(6)	177.8(5)	174(2)	174.2(9)	176.0(9)
O1-C4-C5-C6 torsion (°)	-178.8	-175.7(4)	-175.9(4)	-176(2)	-175.5(7)	-181.4(8)

Table 9. *A comparison of the refined structural parameters for acetaminophen between the data taken on a pure sample, and one composed of only 38% acetaminophen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Acetaminophen			**39% Acetaminophen**		
	Haisa (1976)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	12.93	12.8861(2)	12.8856(2)	12.884(2)	12.8887(4)	12.8869(6)
b(Å)	9.40	9.3812(1)	9.3801(1)	9.382(1)	9.3840(3)	9.3833(4)
c(Å)	7.10	7.1010(1)	7.1010(1)	7.103(1)	7.1025(2)	7.1022(4)
β(°)	115.9	115.7015(8)	115.7002(9)	115.709(8)	115.702(2)	115.706(3)
B (isotropic)		3.14(7)	2.76(7)	5.6(9)	4.0(2)	3.7(3)
aromatic(Å)	1.388	1.387(2)	1.382(2)	1.40(2)	1.377(5)	1.406(6)
N1-C1 bond (Å)	1.425	1.406(4)	1.411(4)	1.27(5)	1.36(1)	1.42(2)
C7-N1 bond (Å)	1.341	1.337(7)	1.325(7)	1.54(6)	1.35(2)	1.32(3)
O2-C7 bond (Å)	1.232	1.244(7)	1.237(7)	1.20(7)	1.21(2)	1.18(3)
C8-C7 bond (Å)	1.509	1.507(7)	1.505(6)	1.84(7)	1.55(2)	1.62(3)
O1-C4 bond (Å)	1.377	1.391(4)	1.402(4)	1.59(5)	1.46(1)	1.47(2)
x		16.5347(2)	16.5345(2)	16.528(3)	16.5313(8)	16.529(1)
y		8.2627(3)	8.2629(2)	8.251(2)	8.2620(8)	8.2601(9)
z		-0.0777(4)	-0.0784(3)	-0.092(3)	-0.074(1)	-0.086(1)
Rotation around x (°)		-227.4(1)	-227.5(1)	-225(1)	-228.2(4)	-223.7(4)
Rotation around y (°)		199.3(2)	199.4(2)	204(2)	200.8(6)	202.2(6)
Rotation around z (°)		-219.3(2)	-219.4(2)	-221(2)	-219.9(6)	-223.5(7)
N1-C1-C2 angle (°)	124.3	121.4(5)	121.7(5)	131(6)	120(2)	132(2)
C7-N1-C1 angle (°)	128.2	132.4(7)	131.8(6)	106(6)	135(2)	113(2)
O2-C7-N1 angle (°)	122.8	121.4(7)	122.0(6)	132(7)	120(2)	138(3)
C8-C7-N1 angle (°)	114.69	119.3(5)	119.1(5)	114(5)	118(2)	109(2)
O1-C4-C5 angle (°)	117.7	120.4(5)	120.6(4)	132(5)	125(2)	132(2)
N1-C1-C2-C3 torsion (°)	179.8	179.3(5)	178.9(4)	154(7)	178(2)	175(2)
C7-N1-C1-C2 torsion (°)	23.4	20.4(9)	21.7(8)	50(8)	16(3)	24(3)
O2-C7-N1-C1 torsion (°)	-2.2	3(1)	1(1)	-37(12)	11(4)	10(5)
C8-C7-N1-C1 torsion (°)	177.68	177.4(6)	177.8(5)	161(6)	173(2)	172(2)
O1-C4-C5-C6 torsion (°)	-178.8	-175.7(4)	-175.9(4)	-182(5)	-175(1)	-185(2)

Table 10. *A comparison of the refined structural parameters for acetaminophen between the data taken on a pure sample, and one composed of only 25% acetaminophen. Numbers in parenthesis are the standard errors computed by TOPAS.*

	Pure Acetaminophen			**25% Acetaminophen**		
	Haisa (1976)	Rietveld	Robust	Single Riet.	Dual Riet.	Robust
a(Å)	12.93	12.8861(2)	12.8856(2)	12.656(5)	12.885(2)	12.864(8)
b(Å)	9.40	9.3812(1)	9.3801(1)	9.564(3)	9.386(2)	9.354(5)
c(Å)	7.10	7.1010(1)	7.1010(1)	7.236(2)	7.101(1)	7.104(6)
β(°)	115.9	115.7015(8)	115.7002(9)	117.10(2)	115.71(1)	115.83(5)
B (isotropic)		3.14(7)	2.76(7)	20(3)	25(5)	2(1)
aromatic(Å)	1.388	1.387(2)	1.382(2)	2.57(5)	1.6(6)	1.73(3)
N1-C1 bond (Å)	1.425	1.406(4)	1.411(4)	2.4(1)	1.4(2)	1.05(9)
C7-N1 bond (Å)	1.341	1.337(7)	1.325(7)	4(1)	1.8(3)	1.6(1)
O2-C7 bond (Å)	1.232	1.244(7)	1.237(7)	2(1)	0.9(3)	1.0(1)
C8-C7 bond (Å)	1.509	1.507(7)	1.505(6)	2(1)	2.6(3)	1.8(1)
O1-C4 bond (Å)	1.377	1.391(4)	1.402(4)	3.1(1)	1.6(1)	2.00(6)
x		16.5347(2)	16.5345(2)	16.500(5)	16.541(8)	16.562(4)
y		8.2627(3)	8.2629(2)	8.312(5)	8.264(9)	8.222(3)
z		-0.0777(4)	-0.0784(3)	-0.370(6)	-0.04(2)	-0.116(4)
Rotation around x (°)		-227.4(1)	-227.5(1)	-236(1)	-231(5)	-211(2)
Rotation around y (°)		199.3(2)	199.4(2)	189(1)	2(1)	207(2)
Rotation around z (°)		-219.3(2)	-219.4(2)	-212(2)	-208(10)	-238(2)
N1-C1-C2 angle (°)	124.3	121.4(5)	121.7(5)	179.3(3)	115(34)	166(6)
C7-N1-C1 angle (°)	128.2	132.4(7)	131.8(6)	133(19)	133(31)	108(8)
O2-C7-N1 angle (°)	122.8	121.4(7)	122.0(6)	26(6)	82(38)	99(10)
C8-C7-N1 angle (°)	114.69	119.3(5)	119.1(5)	90(12)	81(16)	128(8)
O1-C4-C5 angle (°)	117.7	120.4(5)	120.6(4)	45(3)	94(20)	136(4)
N1-C1-C2-C3 torsion (°)	179.8	179.3(5)	178.9(4)	190(270)	174(24)	253(30)
C7-N1-C1-C2 torsion (°)	23.4	20.4(9)	21.7(8)	10(270)	5(37)	71(30)
O2-C7-N1-C1 torsion (°)	-2.2	3(1)	1(1)	103(9)	3(52)	-39(11)
C8-C7-N1-C1 torsion (°)	177.68	177.4(6)	177.8(5)	107(8)	201(30)	158(11)
O1-C4-C5-C6 torsion (°)	-178.8	-175.7(4)	-175.9(4)	-208(5)	-128(21)	-153(6)