

Table 1S The unit cell parameters for polymorphs I, II, and III of tolbutamide.

<i>T</i> / K	<i>a</i> / Å	<i>b</i> / Å	<i>c</i> / Å	β / °	<i>V</i> / Å ³
Form I ^L (Space group <i>Pna</i> 2 ₁)					
100	19.4331(3)	7.8010(1)	9.0277(1)	90	1368.58(3)
125	19.5258(4)	7.7980(2)	9.0393(2)	90	1376.35(8)
150	19.5903(4)	7.8037(2)	9.0437(2)	90	1382.58(9)
175	19.6761(7)	7.7996(2)	9.0454(3)	90	1388.2(1)
200	19.7525(3)	7.7998(1)	9.0583(1)	90	1395.58(7)
225	19.8557(7)	7.8007(3)	9.0583(2)	90	1403.0(1)
250	19.965(1)	7.8083(4)	9.0614(4)	90	1412.6(2)
275	20.1019(8)	7.8163(3)	9.0760(3)	90	1426.0(1)
295	20.2133(6)	7.8233(2)	9.0717(2)	90	1434.55(6)
310	20.3414(9)	7.8351(3)	9.0731(3)	90	1446.0(1)
Form I ^H (Space group <i>Pna</i> 2 ₁)					
320	20.739(10)	7.910(8)	9.063(4)	90	1486(1)
330	20.7500(15)	7.9160(7)	9.0580(5)	90	1487.8(2)
350	20.785(18)	7.950(7)	9.065(5)	90	1498(2)
Form II (Space group <i>Pc</i>)					
100	9.0256(2)	17.1443(5)	17.7904(5)	94.268(3)	2745.2(1)
125	9.040(1)	17.159(3)	17.827(3)	94.50(1)	2756.6(5)
150	9.0536(3)	17.1709(8)	17.8902(7)	94.864(4)	2771.2(2)
175	9.0735(12)	17.190(3)	17.973(3)	95.19(1)	2791.8(6)
200	9.0875(11)	17.192(3)	18.038(3)	95.61(1)	2804.6(6)
225	9.111(3)	17.194(6)	18.108(6)	95.87(3)	2821.8(9)
250	9.118(3)	17.220(3)	18.152(14)	96.02(1)	2834.3(7)
275	9.1245(13)	17.217(3)	18.178(3)	96.14(1)	2839.3(8)
295	9.1371(2)	17.2462(5)	18.2760(5)	96.236(2)	2855.1(1)
Form III ² (Space group <i>P</i> 2 ₁ / <i>n</i>)					
100	11.5671(1)	27.1703(3)	13.5558(2)	102.746(1)	4155.35(8)
125	11.6048(5)	27.160(1)	13.6057(6)	102.968(4)	4179.0(4)
Form III (Space group <i>P</i> 2 ₁ / <i>n</i>)					
150	11.7120(3)	9.0247(1)	13.6984(3)	103.490(2)	1407.94(5)
175	11.7446(5)	9.0383(4)	13.7609(7)	103.676(5)	1419.32(2)
200	11.7520(7)	9.0288(6)	13.796(1)	103.859(7)	1421.5(2)
225	11.7596(8)	9.0320(5)	13.8374(8)	104.009(7)	1426.0(2)
250	11.7762(9)	9.0397(5)	13.886(1)	104.199(7)	1433.1(2)
275	11.7949(9)	9.0425(5)	13.929(1)	104.347(8)	1437.3(2)
295	11.8100(6)	9.0587(3)	13.9713(6)	104.491(5)	1447.1(1)