SUPPLEMENTARY INFORMATION

The orientation matrices of the monoclinic α-**1d** and triclinic ß-**1d** are

α-**1d**			ß-**1d**		
-0.04498	0.03470	-0.05025	0.09575	0.00268	0.00270
0.01226	0.04616	0.04715	0.01456	0.04294	-0.08065
0.05998	0.01658	-0.02612	-0.04025	0.08283	0.00623

The phase transformation is described by matrices

α-**1d**	ß-**1d**		α-**1d**	ß-**1d**	
-1/2	1/2	-1/2	-1	1	0
1/2	1/2	-1/2	1	1	-1
0	0	-1	0	0	-1

which give the calculated orientation matrices

for α-**1d**			for ß-**1d**		
-0.04654	0.04922	-0.05192	0.07965	-0.01028	0.01556
0.01419	0.02876	0.05189	0.03390	0.05844	-0.09332
0.06154	0.02129	-0.02752	-0.04340	0.07656	0.00953

(note that the crystal tilted on its mount during the phase transition; this may in part account for the discrepancy between the calculated and measured orientation matrices)

The ß-**1d** unit cell calculated from the transformation matrix is

a=11.924, *b*=13.598, *c*=13.936, α =51.28, ß =62.88, γ=63.57;

cf. the measured one of

a=10.209, *b*=12.334, *c*=13.904, α =63.78, ß =74.73, γ=70.54