Table S1. Compatibility of the translation symmetry elements $S = (\mathbf{I}|\mathbf{s})$ with the 23 different tilt systems given by Glazer (1972) and their space group variants. The first column gives the space group and number given by Howard and Stokes (1998). An asterisk indicates that the tilt system has a higher symmetry than that required by the space group, and is therefore not in their main list of isotropy subgroups of Pm3m. The second column gives the number and tilt system from Glazer (1972). The third column gives the 6-vector $\boldsymbol{\tau} = [\mathbf{t}_{[000]}: \mathbf{t}_{[111]}]$ used in this work.

Symmetry element $S = (\mathbf{I} \mid \mathbf{s})$

Howard & Stokes		Glazer		6-vector	s							
					[000]	[001]	[010]	[100]	[011]	[101]	[110]	[111]
1	*Pm m* (#221)	23	$a^0a^0a^0$	0,0,0: 0,0,0	✓	✓	✓	✓	✓	✓	✓	✓
6	*I4/mcm* (#140)	22	$a^0a^0c^-$	0,0,*c*: 0,0,-*c*	✓				✓	✓	✓	
				0,*b*,0: 0,-*b*,0	✓				✓	✓	✓	
				a,0,0: -*a*,0,0	✓				✓	✓	✓	
2	*P4/mbm* (#127)	21	$a^0a^0c^+$	0,0,*c*: 0,0,*c*	✓	✓					✓	✓
				0,*b*,0: 0,*b*,0	✓		✓			✓		✓
				a,0,0: *a*,0,0	✓			✓	✓			✓
7	*Imma* (#74)	20	$a^0b^-b^-$	0,*b*,*b*: 0,-*b*,-*b*	✓				✓	✓	✓	
				0,*b*,-*b*: 0,-*b*,*b*	✓				✓	✓	✓	
				a,0,*a*: -*a*,0,-*a*	✓				✓	✓	✓	
				a,0,-*a*: -*a*,0,*a*	✓				✓	✓	✓	
				a,*a*,0: -*a*,-*a*,0	✓				✓	✓	✓	
				a,-*a*,0: -*a*,*a*,0	✓				✓	✓	✓	
9	*C2/m* (#12)	19	$a^0b^-c^-$	0,*b*,*c*: 0,-*b*,-*c*	✓				✓	✓	✓	
				a,0,*c*: -*a*,0,-*c*	✓				✓	✓	✓	
				a,*b*,0: -*a*,-*b*,0	✓				✓	✓	✓	
* (12)	* *Cmcm* (#63)	18	$a^0b^+b^-$	0,*b*,*b*: 0,*b*,-*b*	✓					✓		
				0,*b*,*b*: 0,-*b*,*b*	✓						✓	
				a,0,*a*: *a*,0,-*a*	✓				✓			
				a,0,*a*: -*a*,0,*a*	✓						✓	
				a, *a*,0: *a*,-*a*,0	✓				✓			
				a, *a*,0: -*a*,*a*,0	✓					✓		
12	*Cmcm* (#63)	17	$a^0b^+c^-$	0,*b*,*c*: 0,*b*,-*c*	✓					✓		
				0,*b*,*c*: 0,-*b*,*c*	✓						✓	
				a,0,*c*: *a*,0,-*c*	✓				✓			
				a,0,*c*: -*a*,0,*c*	✓						✓	
				a,*b*,0: *a*,-*b*,0	✓				✓			
				a,*b*,0: -*a*,*b*,0	✓					✓		
3	*I4/mmm* (#139)	16	$a^0b^+b^+$	0,*b*,*b*: 0,*b*,*b*	✓							✓
				0,*b*,-*b*:0,*b*,-*b*	✓							✓
				a,0,*a*: *a*,0,*a*	✓							✓
				a,0,-*a*: *a*,0,-*a*	✓							✓
				a,*a*,0: *a*,*a*,0	✓							✓
				a,-*a*,0: *a*,-*a*,0	✓							✓
*(5)	* *Immm* (#71)	15	$a^0b^+c^+$	0,*b*,*c*: 0,*b*,*c*	✓							✓
8	*R c* (#167)	14	$a^-a^-a^-$	*a*,*a*,*a*: -*a*,-*a*,-*a*	✓				✓	✓	✓	
				a,*a*,-*a*: -*a*,-*a*,*a*	✓				✓	✓	✓	
				a,-*a*,*a*: -*a*,*a*,-*a*	✓				✓	✓	✓	

			a,-a,-a: -*a,a,a*	✓				✓	✓	✓	
10	*C*2/*c* (#15)	13	$a^-b^-b^-$	*a,b,b*: -*a,-b,-b*	✓				✓	✓	✓	
				a,b,-b: -*a,-b,b*	✓				✓	✓	✓	
				a,b,a: -*a,-b,-a*	✓				✓	✓	✓	
				a,b,-a: -*a,-b,a*	✓				✓	✓	✓	
				a,a,c: -*a,-a,-c*	✓				✓	✓	✓	
				a,-a,c: -*a,a,-c*	✓				✓	✓	✓	
11	*P* (#2)	12	$a^-b^-c^-$	*a,b,c*: -*a,-b,-c*	✓				✓	✓	✓	
*	*	11	$a^+a^-a^-$	*a,a,a*: *a,-a,-a*	✓				✓			
				a,a,-a: *a,-a,a*	✓				✓			
(13)	*Pnma* (#62)			*a,a,a*: -*a,a,-a*	✓					✓		
				a,a,-a: -*a,a,a*	✓					✓		
				a,a,a: -*a,-a,a*	✓						✓	
				a,-a,a: -*a,a,a*	✓						✓	
13	*Pnma* (#62)	10	$a^+b^-b^-$	*a,b,b*: *a,-b,-b*	✓				✓			
				a,b,-b: *a,-b,b*	✓				✓			
				a,b,a: -*a,b,-a*	✓					✓		
				a,b,-a: -*a,b,a*	✓					✓		
				a,a,c: -*a,-a,c*	✓						✓	
				a,-a,c: -*a,a,c*	✓						✓	
*	*	9	$a^+a^-c^-$	*a,a,c*: *a,-a,-c*	✓				✓			
				a,b,b: -*a,b,-b*	✓					✓		
(14)	$P2_1/m$ (#11)			*a,b,a*: -*a,-b,a*	✓						✓	
14	$P2_1/m$ (#11)	8	$a^+b^-c^-$	*a,b,c*: *a,-b,-c*	✓				✓			
				a,b,c: -*a,b,-c*	✓					✓		
				a,b,c: -*a,-b,c*	✓						✓	
*	*	7	$a^+a^+a^-$	*a,a,a*: *a,a,-a*	✓							
				a,-a,a: *a,-a,-a*	✓							
(15)	$P4_2/nmc$ (#137)			*a,a,a*: *a,-a,a*	✓							
				a,a,-a: *a,-a,-a*	✓							
				a,a,a: -*a,a,a*	✓							
				a,a,-a: -*a,a,-a*	✓							
*	*	6	$a^+b^+b^-$	*a,b,b*: *a,b,-b*	✓							
				a,b,a: *a,b,-a*	✓							
*	*Pmmn* (#59)			*a,a,c*: *a,-a,c*	✓							
15	$P4_2/nmc$ (#137)	5	$a^+a^+c^-$	*a,a,c*: *a,a,-c*	✓							
				a,-a,c: *a,-a,-c*	✓							
				a,b,a: *a,-b,a*	✓							
				a,b,-a: *a,-b,-a*	✓							
				a,b,b: -*a,b,b*	✓							
				a,b,-b: -*a,b,-b*	✓							
*	*	4	$a^+b^+c^-$	*a,b,c*: *a,b,-c*	✓							
				a,b,c: *a,-b,c*	✓							
*	*Pmmn* (#59)			*a,b,c*: -*a,b,c*	✓							
4	*Im*	3	$a^+a^+a^+$	*a,a,a*: *a,a,a*	✓							✓
				a,a,-a: *a,a,-a*	✓							✓
				a,-a,a: *a,-a,a*	✓							✓
				a,-a,-a: *a,-a,-a*	✓							✓
*	* *Immm* (#71)	2	$a^+b^+b^+$	*a,b,b*: *a,b,b*	✓							✓
				a,b,a: *a,b,a*	✓							✓
				a,a,c: *a,a,c*	✓							✓
5	*Immm* (#71)	1	$a^+b^+c^+$	*a,b,c*: *a,b,c*	✓							✓

Table S2. Compatibility of the mirror symmetry elements $S = (m_{yz}|\mathbf{s})$ with the 23 different tilt systems given by Glazer (1972) and their space group variants.

Symmetry element $S = (m_{yz} \mid \mathbf{s})$

Howard & Stokes		Glazer		6-vector	s							
					[000]	[001]	[010]	[100]	[011]	[101]	[110]	[111]
1	*Pm m* (#221)	23	$a^0a^0a^0$	0,0,0: 0,0,0	✓	✓	✓	✓	✓	✓	✓	✓
6	*I4/mcm* (#140)	22	$a^0a^0c^-$	0,0,*c*: 0,0,-*c*								
				0,*b*,0: 0,-*b*,0								
				a,0,0: -*a*,0,0		✓	✓	✓				✓
2	*P4/mbm* (#127)	21	$a^0a^0c^+$	0,0,*c*: 0,0,*c*								
				0,*b*,0: 0,*b*,0								
				a,0,0: *a*,0,0		✓	✓			✓	✓	
7	*Imma* (#74)	20	$a^0b^-b^-$	0,*b*,*b*: 0,-*b*,-*b*	✓				✓	✓	✓	
				0,*b*,-*b*: 0,-*b*,*b*		✓	✓	✓				✓
				a,0,*a*: -*a*,0,-*a*								
				a,0,-*a*: -*a*,0,*a*								
				a,*a*,0: -*a*,-*a*,0								
				a,-*a*,0: -*a*,*a*,0								
9	*C2/m* (#12)	19	$a^0b^-c^-$	0,*b*,*c*: 0,-*b*,-*c*								
				a,0,*c*: -*a*,0,-*c*								
				a,*b*,0: -*a*,-*b*,0								
* (12)	* *Cmcm* (#63)	18	$a^0b^+b^-$	0,*b*,*b*: 0,*b*,-*b*								
				0,*b*,*b*: 0,-*b*,*b*								
				a,0,*a*: *a*,0,-*a*								
				a,0,*a*: -*a*,0,*a*								
				a, *a*,0: *a*,-*a*,0								
				a, *a*,0: -*a*,*a*,0								
12	*Cmcm* (#63)	17	$a^0b^+c^-$	0,*b*,*c*: 0,*b*,-*c*								
				0,*b*,*c*: 0,-*b*,*c*								
				a,0,*c*: *a*,0,-*c*								
				a,0,*c*: -*a*,0,*c*								
				a,*b*,0: *a*,-*b*,0								
				a,*b*,0: -*a*,*b*,0								
3	*I4/mmm* (#139)	16	$a^0b^+b^+$	0,*b*,*b*: 0,*b*,*b*	✓							✓
				0,*b*,-*b*:0,*b*,-*b*				✓	✓			
				a,0,*a*: *a*,0,*a*								
				a,0,-*a*: *a*,0,-*a*								
				a,*a*,0: *a*,*a*,0								
				a,-*a*,0: *a*,-*a*,0								
*(5)	* *Immm* (#71)	15	$a^0b^+c^+$	0,*b*,*c*: 0,*b*,*c*								
8	*R c* (#167)	14	$a^-a^-a^-$	*a*,*a*,*a*: -*a*,-*a*,-*a*								
				a,*a*,-*a*: -*a*,-*a*,*a*		✓	✓	✓				✓
				a,-*a*,*a*: -*a*,*a*,-*a*		✓	✓	✓				✓
				a,-*a*,-*a*: -*a*,*a*,*a*								
10	*C2/c* (#15)	13	$a^-b^-b^-$	*a*,*b*,*b*: -*a*,-*b*,-*b*								
				a,*b*,-*b*: -*a*,-*b*,*b*		✓	✓	✓				✓
				a,*b*,*a*: -*a*,-*b*,-*a*								
				a,*b*,-*a*: -*a*,-*b*,*a*								
				a,*a*,*c*: -*a*,-*a*,-*c*								

			a,-a,c: -*a,a,-c*								
11	*P* (#2)	12	$a^-b^-c^-$	*a,b,c*: -*a,-b,-c*								
* (13)	* *Pnma* (#62)	11	$a^+a^-a^-$	*a,a,a*: *a,-a,-a*						✓	✓	
				a,a,-a: *a,-a,a*		✓	✓					
				a,a,a: -*a,a,-a*								
				a,a,-a: -*a,a,a*								
				a,a,a: -*a,-a,a*								
				a,-a,a: -*a,a,a*								
13	*Pnma* (#62)	10	$a^+b^-b^-$	*a,b,b*: *a,-b,-b*						✓	✓	
				a,b,-b: *a,-b,b*		✓	✓					
				a,b,a: -*a,b,-a*								
				a,b,-a: -*a,b,a*								
				a,a,c: -*a,-a,c*								
				a,-a,c: -*a,a,c*								
* (14)	* $P2_1/m$ (#11)	9	$a^+a^-c^-$	*a,a,c*: *a,-a,-c*								
				a,b,b: -*a,b,-b*								
				a,b,a: -*a,-b,a*								
14	$P2_1/m$ (#11)	8	$a^+b^-c^-$	*a,b,c*: *a,-b,-c*								
				a,b,c: -*a,b,-c*								
				a,b,c: -*a,-b,c*								
* (15)	* $P4_2/nmc$ (#137)	7	$a^+a^+a^-$	*a,a,a*: *a,a,-a*								
				a,-a,a: *a,-a,-a*								
				a,a,a: *a,-a,a*								
				a,a,-a: *a,-a,-a*								
				a,a,a: -*a,a,a*								✓
				a,a,-a: -*a,a,-a*				✓				
*	* *Pmmn* (#59)	6	$a^+b^+b^-$	*a,b,b*: *a,b,-b*								
				a,b,a: *a,b,-a*								
				a,a,c: *a,-a,c*								
15	$P4_2/nmc$ (#137)	5	$a^+a^+c^-$	*a,a,c*: *a,a,-c*								
				a,-a,c: *a,-a,-c*								
				a,b,a: *a,-b,a*								
				a,b,-a: *a,-b,-a*								
				a,b,b: -*a,b,b*								✓
				a,b,-b: -*a,b,-b*				✓				
*	* *Pmmn* (#59)	4	$a^+b^+c^-$	*a,b,c*: *a,b,-c*								
				a,b,c: *a,-b,c*								
				a,b,c: -*a,b,c*								
4	*Im*	3	$a^+a^+a^+$	*a,a,a*: *a,a,a*								
				a,a,-a: *a,a,-a*								
				a,-a,a: *a,-a,a*								
				a,-a,-a: *a,-a,-a*								
*	* *Immm* (#71)	2	$a^+b^+b^+$	*a,b,b*: *a,b,b*								
				a,b,a: *a,b,a*								
				a,a,c: *a,a,c*								
5	*Immm* (#71)	1	$a^+b^+c^+$	*a,b,c*: *a,b,c*								

Table S3. Compatibility of the mirror symmetry elements $S = (m_z|\mathbf{s})$ with the 23 different tilt systems given by Glazer (1972) and their space group variants.

Symmetry element $S = (m_z \mid \mathbf{s})$

Howard & Stokes		Glazer		6-vector	**s**							
					[000]	[001]	[010]	[100]	[011]	[101]	[110]	[111]
1	*Pm m* (#221)	23	$a^0a^0a^0$	0,0,0: 0,0,0	✓	✓	✓	✓	✓	✓	✓	✓
6	*I4/mcm* (#140)	22	$a^0a^0c^-$	0,0,*c*: 0,0,-*c*	✓				✓	✓	✓	
				0,*b*,0: 0,-*b*,0		✓	✓	✓				✓
				a,0,0: -*a*,0,0		✓	✓	✓				✓
2	*P4/mbm* (#127)	21	$a^0a^0c^+$	0,0,*c*: 0,0,*c*	✓	✓					✓	✓
				0,*b*,0: 0,*b*,0		✓		✓	✓		✓	
				a,0,0: *a*,0,0		✓	✓			✓	✓	
7	*Imma* (#74)	20	$a^0b^-b^-$	0,*b*,*b*: 0,-*b*,-*b*								
				0,*b*,-*b*: 0,-*b*,*b*								
				a,0,*a*: -*a*,0,-*a*								
				a,0,-*a*: -*a*,0,*a*								
				a,*a*,0: -*a*,-*a*,0		✓	✓	✓				✓
				a,-*a*,0: -*a*,*a*,0		✓	✓	✓				✓
9	*C2/m* (#12)	19	$a^0b^-c^-$	0,*b*,*c*: 0,-*b*,-*c*								
				a,0,*c*: -*a*,0,-*c*								
				a,*b*,0: -*a*,-*b*,0		✓	✓	✓				✓
* (12)	* *Cmcm* (#63)	18	$a^0b^+b^-$	0,*b*,*b*: 0,*b*,-*b*					✓		✓	
				0,*b*,*b*: 0,-*b*,*b*		✓						✓
				a,0,*a*: *a*,0,-*a*						✓	✓	
				a,0,*a*: -*a*,0,*a*		✓						✓
				a, *a*,0: *a*,-*a*,0		✓	✓					
				a, *a*,0: -*a*,*a*,0		✓		✓				
12	*Cmcm* (#63)	17	$a^0b^+c^-$	0,*b*,*c*: 0,*b*,-*c*					✓		✓	
				0,*b*,*c*: 0,-*b*,*c*		✓						✓
				a,0,*c*: *a*,0,-*c*						✓	✓	
				a,0,*c*: -*a*,0,*c*		✓						✓
				a,*b*,0: *a*,-*b*,0		✓	✓					
				a,*b*,0: -*a*,*b*,0		✓		✓				
3	*I4/mmm* (#139)	16	$a^0b^+b^+$	0,*b*,*b*: 0,*b*,*b*		✓					✓	
				0,*b*,-*b*:0,*b*,-*b*		✓					✓	
				a,0,*a*: *a*,0,*a*		✓					✓	
				a,0,-*a*: *a*,0,-*a*		✓					✓	
				a,*a*,0: *a*,*a*,0		✓					✓	
				a,-*a*,0: *a*,-*a*,0		✓					✓	
*(5)	* *Immm* (#71)	15	$a^0b^+c^+$	0,*b*,*c*: 0,*b*,*c*		✓					✓	
8	*R c* (#167)	14	$a^-a^-a^-$	*a*,*a*,*a*: -*a*,-*a*,-*a*								
				a,*a*,-*a*: -*a*,-*a*,*a*								
				a,-*a*,*a*: -*a*,*a*,-*a*								
				a,-*a*,-*a*: -*a*,*a*,*a*								
10	*C2/c* (#15)	13	$a^-b^-b^-$	*a*,*b*,*b*: -*a*,-*b*,-*b*								
				a,*b*,-*b*: -*a*,-*b*,*b*								
				a,*b*,*a*: -*a*,-*b*,-*a*								
				a,*b*,-*a*: -*a*,-*b*,*a*								
				a,*a*,*c*: -*a*,-*a*,-*c*								

			a,-a,c: -*a,a,-c*								
11	*P* (#2)	12	$a^-b^-c^-$	*a,b,c*: -*a,-b,-c*								
* (13)	* *Pnma* (#62)	11	$a^+a^-a^-$	*a,a,a*: *a,-a,-a*								
				a,a,-a: *a,-a,a*								
				a,a,a: -*a,a,-a*								
				a,a,-a: -*a,a,a*								
				a,a,a: -*a,-a,a*		✓						✓
				a,-a,a: -*a,a,a*		✓						✓
13	*Pnma* (#62)	10	$a^+b^-b^-$	*a,b,b*: *a,-b,-b*								
				a,b,-b: *a,-b,b*								
				a,b,a: -*a,b,-a*								
				a,b,-a: -*a,b,a*								
				a,a,c: -*a,-a,c*		✓						✓
				a,-a,c: -*a,a,c*		✓						✓
* (14)	* $P2_1/m$ (#11)	9	$a^+a^-c^-$	*a,a,c*: *a,-a,-c*								
				a,b,b: -*a,b,-b*								
				a,b,a: -*a,-b,a*		✓						✓
14	$P2_1/m$ (#11)	8	$a^+b^-c^-$	*a,b,c*: *a,-b,-c*								
				a,b,c: -*a,b,-c*								
				a,b,c: -*a,-b,c*		✓						✓
* (15)	* $P4_2/nmc$ (#137)	7	$a^+a^+a^-$	*a,a,a*: *a,a,-a*							✓	
				a,-a,a: *a,-a,-a*							✓	
				a,a,a: *a,-a,a*		✓						
				a,a,-a: *a,-a,-a*		✓						
				a,a,a: -*a,a,a*		✓						
				a,a,-a: -*a,a,-a*		✓						
*	* *Pmmn* (#59)	6	$a^+b^+b^-$	*a,b,b*: *a,b,-b*							✓	
				a,b,a: *a,b,-a*							✓	
				a,a,c: *a,-a,c*		✓						
15	$P4_2/nmc$ (#137)	5	$a^+a^+c^-$	*a,a,c*: *a,a,-c*							✓	
				a,-a,c: *a,-a,-c*							✓	
				a,b,a: *a,-b,a*		✓						
				a,b,-a: *a,-b,-a*		✓						
				a,b,b: -*a,b,b*		✓						
				a,b,-b: -*a,b,-b*		✓						
*	* *Pmmn* (#59)	4	$a^+b^+c^-$	*a,b,c*: *a,b,-c*							✓	
				a,b,c: *a,-b,c*		✓						
				a,b,c: -*a,b,c*		✓						
4	*Im*	3	$a^+a^+a^+$	*a,a,a*: *a,a,a*		✓					✓	
				a,a,-a: *a,a,-a*		✓					✓	
				a,-a,a: *a,-a,a*		✓					✓	
				a,-a,-a: *a,-a,-a*		✓					✓	
*	* *Immm* (#71)	2	$a^+b^+b^+$	*a,b,b*: *a,b,b*		✓					✓	
				a,b,a: *a,b,a*		✓					✓	
				a,a,c: *a,a,c*		✓					✓	
5	*Immm* (#71)	1	$a^+b^+c^+$	*a,b,c*: *a,b,c*		✓					✓	