Effects of merohedric twinning on the diffraction pattern. Erratum and corrigenda

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A number of corrections are made to the article by Nespolo *et al.* [*Acta Cryst.* (2014), A**70**, 106–125].

On p. 110, the first sentence of the second paragraph should start as follows: 'Tables 2 to 5 list the 101 merohedral non-symmorphic types of space groups *H* that can give rise to 147 twin laws . . .'

Misalignment of some of the entries the third and fourth columns of Table 3 make this table difficult to read. It is reproduced here with better alignment of the entries in these columns.

In Table 4, the asterisks (*) marking two of the entries in the fifth column should be omitted. The corrected table is given here.

In Table 7, the sixth entry from the bottom of the 13th column, $l = 4n$, should not be bold.

We thank Howard Flack for spotting these errors.

Table 3
Classification of the 34 merohedral non-symmorphic space-group types H in the tetragonal crystal family, which can give rise to 42 twin laws.

Three twin laws (indicated by the symbol {) have been split into two, because two different coset representatives give different results in terms of G, leading to a total of 45 cases. Among these, ten cannot be extended by a twofold operation s corresponding to the twin operation t ('no extension' in the table), and 16 more do have such an extension but none of the corresponding supergroups G has the same reflection conditions as H ('---' in the table). For these 26 cases (16 for class I and ten for class IIA) the **G** model is ruled out on the basis of the observed reflection conditions: H in the corresponding row is shown in bold, accompanied by dashes in the last column. For the other 19 cases, the group $G^{\#}$ having the same reflection conditions as H is given; in the tetragonal crystal family, $G^{\#}$ is always a supergroup of H. Entries are ordered according to the diffraction symbol, as given in LVB.

Diffraction symbol	H	No.	t	$G^{\#}$	No.
Non-centrosymmetric hemihedral (only class I twinning possible)					
$P\text{-}2_1\text{-}$	**$P4_22_12$**	90	$\bar{1}$	---	---
	$P\bar{4}2_1m$	113		---	---
$P4_2\text{--}$	**$P4_222$**	93		---	---
$P4_22_1\text{-}$	**$P4_22_12$**	94		---	---
$P4_1\text{--}$	**$P4_122$**	91		no extension	---
	$P4_322$	95		no extension	---
$P4_12_1\text{--}$	**$P4_12_12$**	92		no extension	---
	$P4_32_12$	96		no extension	---
$P\text{--}c$	$P4_2mc$	105		$P4_2/mmc$	131
	$P\bar{4}2c$	112			
$P\text{-}2_1c$	**$P\bar{4}2_1c$**	114		---	---
$P\text{-}b\text{-}$	$P4bm$	100		$P4/mbm$	127
	$P\bar{4}b2$	117			
$P\text{-}bc$	$P4_2bc$	106		$P4_2/mbc$	135
$P\text{-}c\text{-}$	$P4_2cm$	101		$P4_2/mcm$	132
	$P\bar{4}c2$	116			
$P\text{-}cc$	$P4cc$	103		$P4/mcc$	124
$P\text{-}n\text{-}$	$P4_2nm$	102		$P4_2/mnm$	136
	$P\bar{4}n2$	118			
$P\text{-}nc$	$P4nc$	104		$P4/mnc$	128
$I4_1\text{--}$	**$I4_122$**	98		---	---
$I\text{--}d$	**$I4_1md$**	109		---	---
	$I\bar{4}2d$	122		---	---
$I\text{-}c\text{-}$	$I4cm$	108		$I4/mcm$	140
	$I\bar{4}c2$	120			
$I\text{-}cd$	**$I4_1cd$**	110		---	---
Centrosymmetric hemihedral (only class IIA twinning possible)					
$P4_2\text{--}$	**$P4_2/m$**	84	$2_{[100]}$	---	---
			$2_{[110]}$	no extension	---
$Pn\text{--}$	**$P4/n$**	85	$2_{[100]}$	---	---
			$2_{[110]}$	$P4/nmm$	129
$P4_2/n\text{--}$	**$P4_2/n$**	86	$2_{[100]}$	---	---
Tetartohedral (both class I and class IIA twinning possible)					
$P4_2\text{--}$	**$P4_2$**	77	$\bar{1}$	$P4_2/m$	84
			$2_{[100]}$	$P4_222$	93
			$m_{[100]}$	---	---
$P4_1\text{--}$	**$P4_1$**	76	$\bar{1}$	no extension	---
			$2_{[100]}$	$P4_122$	91
			$m_{[100]}$	no extension	---
	$P4_3$	78	$\bar{1}$	no extension	---
			$2_{[100]}$	$P4_322$	95
			$m_{[100]}$	no extension	---
$I4\text{--}$	**$I4_1$**	80	$\bar{1}$	---	---
			$2_{[100]}$	$I4_122$	98
			$m_{[100]}$	---	---
			$m_{[110]}$	no extension	---
$I4_1/a\text{--}$	**$I4_1/a$**	88	$2_{[100]}$	---	---

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addenda and errata

Table 4
Classification of the 27 merohedral non-symmorphic space-group types H in the hexagonal crystal family, which can give rise to 61 twin laws.

Among these, 29 cannot be extended by a twofold operation s corresponding to the twin operation t ('no extension' in the table), and two more have such an extension but none of the corresponding supergroups G has the same reflection conditions as H ('---' in the table): for these 31 cases (15 for class I and 16 for class IIA) the G model is ruled out on the basis of the observed reflection conditions: H in the corresponding row is shown in bold, accompanied by dashes in the last column. For the other 30 cases, the group $G^{\#}$ having the same reflection conditions as H is given. Entries are ordered according to the diffraction symbol, as given in LVB.

Diffraction symbol	H	No.	t	$G^{\#}$	No.
Non-centrosymmetric hemihedral (only class I twinning possible)					
P--c	$P6_3mc$	186	$\bar{1}$	$P6_3/mmc$	194
	$P\bar{6}2c$	190			
P-c-	$P6_3cm$	185		$P6_3/mcm$	193
	$P\bar{6}c2$	188			
R-c	$R3c$	161		$R\bar{3}c$	167
$P6_3$--	**$P6_322$**	**182**		**---**	**---**
$P6_2$--	**$P6_222$**	**180**		**no extension**	**---**
	$P6_422$	**181**		**no extension**	**---**
$P6_1$--	**$P6_122$**	**178**		**no extension**	**---**
	$P6_522$	**179**		**no extension**	**---**
P-cc	$P6cc$	184		$P6/mcc$	192
Centrosymmetric hemihedral (only class IIA twinning possible)					
$P6_3$--	**$P6_3/m$**	**176**	$m_{[100]}$	**---**	**---**
P--c	$P\bar{3}1c$	163	$m_{[001]}$	$P6_3/mmc$	194
P-c-	$P\bar{3}c1$	165	$m_{[001]}$	$P6_3/mcm$	193
Tetartohedral or ogdohedral (both class I and class IIA twinning possible)					
$P3_1$--	**$P3_1$**	**144**	$\bar{1}$	**no extension**	**---**
			$2_{[210]}$	$P3_112$	151
			$2_{[100]}$	$P3_121$	152
			$2_{[001]}$	$P6_4$	172
			$m_{[001]}$	**no extension**	**---**
			$m_{[100]}$	**no extension**	**---**
			$m_{[210]}$	**no extension**	**---**
	$P3_112$	**151**	$\bar{1}$	**no extension**	**---**
			$2_{[001]}$	$P6_422$	181
			$m_{[001]}$	**no extension**	**---**
	$P3_121$	**152**	$\bar{1}$	**no extension**	**---**
			$2_{[001]}$	$P6_422$	181
			$m_{[001]}$	**no extension**	**---**
	$P3_2$	**145**	$\bar{1}$	**no extension**	**---**
			$2_{[210]}$	$P3_212$	153
			$2_{[100]}$	$P3_221$	154
			$2_{[001]}$	$P6_2$	171
			$m_{[001]}$	**no extension**	**---**
			$m_{[100]}$	**no extension**	**---**
			$m_{[210]}$	**no extension**	**---**
	$P3_212$	**153**	$\bar{1}$	**no extension**	**---**
			$2_{[001]}$	$P6_222$	180
			$m_{[001]}$	**no extension**	**---**
	$P3_221$	**154**	$\bar{1}$	**no extension**	**---**
			$2_{[001]}$	$P6_222$	180
			$m_{[001]}$	**no extension**	**---**
P--c	$P31c$	159	$\bar{1}$	$P\bar{3}1c$	163
			$m_{[001]}$	$P\bar{6}2c$	190
			$2_{[001]}$	$P6_3mc$	186
P-c-	$P3c1$	158	$\bar{1}$	$P\bar{3}c1$	165
			$m_{[001]}$	$P\bar{6}c2$	188
			$2_{[001]}$	$P6_3cm$	185
$P6_3$--	**$P6_3$**	**173**	$\bar{1}$	$P6_3/m$	176
			$2_{[100]}$	$P6_322$	182
			$m_{[100]}$	**no extension**	**---**
$P6_2$--	**$P6_2$**	**171**	$\bar{1}$	**no extension**	**---**
			$2_{[100]}$	$P6_222$	180
			$m_{[100]}$	**no extension**	**---**
	$P6_4$	**172**	$\bar{1}$	**no extension**	**---**
			$2_{[100]}$	$P6_422$	181
			$m_{[100]}$	**no extension**	**---**
$P6_1$--	**$P6_1$**	**169**	$\bar{1}$	**no extension**	**---**
			$2_{[100]}$	$P6_122$	178
			$m_{[100]}$	**no extension**	**---**
	$P6_5$	**170**	$\bar{1}$	**no extension**	**---**
			$2_{[100]}$	$P6_522$	179
			$m_{[100]}$	**no extension**	**---**