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Verification of a method for determining the degree of crystallinity using experimental and computer-generated powder diffraction patterns. Corrigendum

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An erroneous equation and some values of related parameters in the paper by Toraya [*J. Appl. Cryst.* (2023), **56**, 1751–1763] are corrected.

In the paper by Toraya (2023), the $y(2\theta)^{\rm obs}_{\rm P\_C}$ term in equation (15) on page 1754 should be divided by the disorder factor D, defined as $D = \exp\left[-d(2\sin\theta/\lambda)^2\right]$. It was, however, multiplied with D. The correct equation is given by

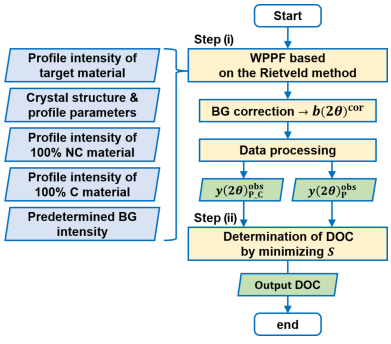
$$y(2\theta)^{\rm obs\_D}_{\rm P\_C} = y(2\theta)^{\rm obs}_{\rm P\_C}\left\{\exp\left[-d\left(\frac{2\sin\theta}{\lambda}\right)^2\right]\right\}^{-1}.$$

Since $\left[\exp\left(-dx^2\right)\right]^{-1} = \exp\left(dx^2\right)$ and d is a variable that is optimized together with the degree of crystallinity, D_0, during

Table 1
Corrected D_0 and d values.

	$\rm DOC_{Av}$ (%)									
	Non-corrected halo pattern					Corrected halo pattern				
$w_{\rm C}$:$w_{\rm NC}$	2:8	4:6	6:4	8:2	Av.	2:8	4:6	6:4	8:2	Av.
E	19.28	38.40	57.97	78.00	1.59	19.28	38.47	57.87	77.58	1.70
	19.30	38.52	58.11	78.10	1.49	19.29	38.54	58.01	77.90	1.57
C	18.93	38.69	58.51	78.52	1.34	18.87	38.58	58.37	78.21	1.49
	18.93	38.77	58.61	78.62	1.27	18.88	38.68	58.54	78.45	1.36
C-p100	20.51	41.29	62.57	84.07	2.11	20.36	40.94	61.75	82.68	1.43
	20.43	41.18	62.07	83.05	1.68	20.41	41.05	61.88	82.78	1.53
C-p50	20.22	40.66	61.87	82.66	1.35	19.99	40.17	60.47	80.96	0.40
	20.10	40.43	60.84	81.38	0.69	20.03	40.26	60.59	81.04	0.48
C-p25	19.04	38.23	58.06	77.79	1.72	18.85	37.78	56.77	75.85	2.69
	18.86	37.80	56.78	75.88	2.67	18.88	37.86	56.87	75.96	2.61
G. Av.					1.62					1.54
					1.56					1.51

	Averaged values of disorder parameter ($d \times 10^2$)							
	Non-corrected halo pattern				Corrected halo pattern			
$w_{\rm C}$:$w_{\rm NC}$	2:8	4:6	6:4	8:2	2:8	4:6	6:4	8:2
E	0.191	0.159	0.149	0.140	0.199	0.152	0.158	−0.346
	0.207	0.159	0.168	0.138	0.192	0.159	0.185	0.155
C	0.165	0.149	0.192	0.137	0.166	0.156	0.191	−0.184
	0.164	0.151	0.181	0.146	0.165	0.166	0.195	0.122
C-p100	0.191	0.190	1.537	2.272	0.201	0.169	0.301	0.178
	0.194	0.160	0.339	0.150	0.194	0.166	0.321	0.180
C-p50	0.229	0.194	2.939	2.443	0.225	0.136	0.104	0.184
	0.230	0.201	0.265	0.180	0.217	0.160	0.254	0.180
C-p25	0.162	0.770	3.438	3.739	0.167	0.149	0.114	0.076
	0.166	0.150	0.113	0.191	0.167	0.145	0.114	0.159



the minimization of the cost function S [equation (22)], the only consequence of this error is considered to be essentially the change of the sign of d from plus to minus and *vice versa*. The D_0 and d values were recalculated for all intensity datasets used in the study, and their correct values are given in Table 1. As was expected, large negative values of d in Table 2 of Toraya (2023) were converted to relatively large positive values in Table 1 of the present article. Large downward deviations of d values from the horizontal line with $d \approx 0$ in Fig. 7 of Toraya (2023) were converted to upward deviations after the recalculation. The influences of other, small d values were negligible, since, for example, $D = 1.0010 \pm 0.0004$ for $2\theta = 80^\circ$ when $d = \mp 0.2 \times 10^{-2}$. The grand averages for the deviations of the derived D_0 values from the nominal values were almost unchanged between the two calculations.

References

Toraya, H. (2023). *J. Appl. Cryst.* **56**, 1751–1763.