addenda and errata



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3DBVSMAPPER: a program for automatically generating bond-valence sum landscapes. Corrigendum

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An equation in the article by Sale & Avdeev [J. Appl. Cryst. (2012), 45, 1054–1056] is corrected.

In the article by Sale & Avdeev (2012), some of the brackets in equation (2) are misplaced. Equation (2) in the original article reads as follows:

$$BVEL_{+/-} = \sum_{j=1}^{N} \left(m_j D_0 \{ \exp[\alpha (R_{\min} - d_j)] - 1 \}^2 - 1 \right).$$
(2)

This should be changed to the following:

$$BVEL_{+/-} = \sum_{j=1}^{N} \left[m_j D_0 \left(\left\{ \exp\left[\alpha \left(R_{\min} - d_j\right)\right] - 1\right\}^2 - 1 \right) \right].$$
(2)

The original code does not have this problem. Therefore, the figures and calculated results are not affected.

References

Sale, M. & Avdeev, M. (2012). J. Appl. Cryst. 45, 1054-1056.



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