The structure of Na₂Y(MoO₄)(PO₄). Corrigendum. By Richard E. Marsh, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, CA 91125, USA

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Abstract
The structure of Na₂Y(MoO₄)(PO₄) was described [Ben Amara & Dabbabi (1987). Acta Cryst. C43, 616–618] as monoclinic, space group C2/c, with a = 13.928 (11), b = 18.016 (10), c = 6.847 (6) Å, β = 119–62 (6)°, Z = 8. It should be described as orthorhombic, space group Ibca. The vectors (010), (101), (001) describe a body-centered cell with a' = 18.016, b' = 12.108, c' = 6.847 Å, α' = 89–83, β' = γ' = 90°, Z = 8; the corresponding coordinate transformations are x' = y, y' = x, z' = x - z.

The Ibca coordinates, after appropriate averaging of equivalent atoms, are given in Table 1. None of the original C2/c coordinates needs to be shifted by more than 2 e.s.d.'s to achieve the symmetry of Ibca; indeed, the r.m.s. value of the shift-to-sigma ratio is 0.8, somewhat below the expectation 0(2,4) 0(5,6) value of 1.0. On the other hand, the angle α' differs from its expectation value of 90° by nearly 3 e.s.d.'s (assuming that the e.s.d. of 0.06° assigned to the original angle β would also apply to the new angle). It is by no means unusual that the e.s.d.'s assigned to unit-cell dimensions do not adequately represent the accuracies of these values; as normally derived, they are estimates of precision only.

Table 1. Coordinates, space group Ibca.

<table>
<thead>
<tr>
<th></th>
<th>x'</th>
<th>y'</th>
<th>z'</th>
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<tbody>
<tr>
<td>Na(1,2)</td>
<td>0.5974 (2)</td>
<td>0.1876 (3)</td>
<td>-0.2646 (5)</td>
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<tr>
<td>Y</td>
<td>0.75</td>
<td>0.07186 (4)</td>
<td>-0.25</td>
</tr>
<tr>
<td>Mo(1,2)</td>
<td>0.3717 (2)</td>
<td>0.1020 (2)</td>
<td>-0.1752 (4)</td>
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<tr>
<td>P</td>
<td>0.4818 (3)</td>
<td>0.1174 (4)</td>
<td>-0.2072 (7)</td>
</tr>
<tr>
<td>O(1)</td>
<td>0.1811 (1)</td>
<td>0.1174 (3)</td>
<td>-0.4596 (6)</td>
</tr>
<tr>
<td>O(2)</td>
<td>0.2416 (2)</td>
<td>0.0152 (5)</td>
<td>-0.5593 (6)</td>
</tr>
<tr>
<td>O(5)</td>
<td>0.07186 (4)</td>
<td>-0.25</td>
<td>-0.2072 (7)</td>
</tr>
<tr>
<td>O(7)</td>
<td>0.2564 (3)</td>
<td>0.0152 (5)</td>
<td>-0.5593 (6)</td>
</tr>
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