| $Tl_3[BO_3]$ | *hP*14 | (176) $P6_3/m$ – $h^2c$ |
|---|---|---|

**$Tl_3BO_3$** [2]
Structural features: $BO_3$ trigonal units in a Mg-type (h.c.p.) arrangement; Tl forms coplanar triangle-mesh layers.

Verbaere A. et al. (1978) [1]
$BO_3Tl_3$
$a = 0.9275$, $c = 0.3775$ nm, $c/a = 0.407$, $V = 0.2812$ nm$^3$, $Z = 2$

| site | Wyck. | sym. | *x* | *y* | *z* | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| O1 | 6*h* | *m*.. | 0.1593 | 0.5898 | $^1/_4$ | | single atom B |
| Tl2 | 6*h* | *m*.. | 0.3551 | 0.0588 | $^1/_4$ | | non-coplanar triangle $O_3$ |
| B3 | 2*c* | -6.. | $^1/_3$ | $^2/_3$ | $^1/_4$ | | coplanar triangle $O_3$ |

Transformation from published data: origin shift 0 0 $^1/_2$

Remarks: Electrostatic model; the position of the Tl electron lone-pair was determined from the evaluation of the electrical field at the Tl(I) nucleus.

References: [1] Verbaere A., Marchand R., Tournoux M. (1978), J. Solid State Chem. 23, 383-390. [2] Marchand R., Piffard Y., Tournoux M. (1973), C. R. Seances Acad. Sci., Ser. C 276, 177-179.