



Fig. 1. Projection of the molecule along the  $y$  axis.

The atomic coordinates are given in Table 1 and bond distances and angles and selected torsion angles in Table 2. Fig. 1 gives a view of the structure with the atomic numbering.

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**Tl<sub>3</sub>{Tl<sub>0.5</sub>(H<sub>3</sub>O)<sub>0.5</sub>}H<sub>14</sub>(PO<sub>4</sub>)<sub>8</sub>·4H<sub>2</sub>O: corrigendum.** By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics,\* California Institute of Technology, Pasadena, California 91125, USA*

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#### Abstract

The structure of this mixed-valence thallium compound (Chiadmi, Vicat, Tran Qui & Boudjada, 1985) was described as triclinic, space group  $P\bar{1}$ , with  $a = 9.820$  (8),  $b = 9.973$  (6),  $c = 17.87$  (1) Å,  $\alpha = 90.14$  (2),  $\beta = 90.01$  (1),  $\gamma = 119.46$  (4)°,  $Z = 2$ . It should be described as monoclinic, space group  $C2/c$ . The vectors (120),  $(\bar{1}00)$ , (001) describe a C-centered cell with  $a' = 17.367$ ,  $b' = 9.820$ ,  $c' = 17.87$  Å,  $\alpha' = 89.99$ ,  $\beta' = 90.17$ ,  $\gamma' = 90.03$ °,  $Z = 4$ ; the correspond-

ing transformations  $x' = \frac{1}{2}y, y' = -x + \frac{1}{2}y, z' = z$  yield coordinates that are consistent with  $C2/c$  within the reported e.s.d.'s. The  $C2/c$  coordinates are given.

Chiadmi *et al.* (1985) noted that the structure is strikingly similar to that of  $(\text{H}_3\text{O})[\text{Al}_3(\text{H}_2\text{PO}_4)_6(\text{HPO}_4)_2] \cdot 4\text{H}_2\text{O}$  (Brodalla & Kniep, 1980). The two compounds are, indeed, isostructural. In the aluminium compound [ $C2/c$ ;  $a = 16.722$  (4),  $b = 9.437$  (6),  $c = 17.126$  (5) Å,  $\beta = 90.87$  (2)°] the  $\text{H}_3\text{O}^+$  ion is the sole occupant of the site labeled T1 in Table 1; in the thallium compound this site is shared equally by Tl and  $\text{H}_3\text{O}^+$ .

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Table 1. Coordinates ( $\times 10^4$  for Tl and P,  $\times 10^3$  for O), space group  $C2/c$ 

Numbers in brackets are shifts in the transformed  $P\bar{1}$  coordinates (Chiadmi *et al.*, 1985) of an individual atom necessary to achieve the symmetry of  $C2/c$ ; numbers in parentheses are the corresponding, transformed e.s.d.'s.

|          | $x'$         | $y'$          | $z'$         |
|----------|--------------|---------------|--------------|
| Tl(1)    | 0 [0] (1)    | -6634 [-] (1) | 2500 [1] (1) |
| Tl(2,3)  | 2121 [0] (1) | -246 [0] (1)  | 2581 [1] (1) |
| Tl       | 0 [0] (1)    | -2406 [-] (2) | 2500 [1] (1) |
| P(1,4)   | 1789 [0] (4) | -2943 [1] (7) | 1403 [3] (4) |
| P(2,7)   | 1251 [1] (4) | -4843 [0] (7) | 3605 [4] (4) |
| P(3,5)   | 4461 [1] (4) | -4429 [1] (7) | 1362 [4] (4) |
| P(6,8)   | 3377 [1] (4) | -2409 [0] (7) | 3478 [2] (4) |
| O(11,41) | 248 [0] (1)  | -380 [1] (2)  | 158 [2] (1)  |
| O(12,43) | 155 [0] (1)  | -191 [1] (2)  | 197 [0] (1)  |
| O(13,44) | 193 [0] (1)  | -225 [0] (2)  | 64 [0] (1)   |
| O(14,42) | 106 [2] (1)  | -381 [1] (2)  | 121 [1] (1)  |
| O(21,72) | 120 [0] (1)  | -556 [0] (2)  | 436 [1] (1)  |
| O(22,74) | 132 [0] (1)  | -331 [1] (2)  | 384 [1] (1)  |
| O(23,71) | 50 [0] (1)   | -498 [1] (2)  | 318 [0] (1)  |

Table 1 (cont.)

|          | $x'$        | $y'$         | $z'$        |
|----------|-------------|--------------|-------------|
| O(24,73) | 196 [0] (1) | -536 [0] (2) | 324 [2] (1) |
| O(31,53) | 525 [0] (1) | -516 [2] (2) | 132 [2] (1) |
| O(32,51) | 417 [1] (1) | -432 [0] (2) | 54 [1] (1)  |
| O(33,52) | 394 [1] (1) | -541 [1] (2) | 176 [2] (1) |
| O(34,54) | 453 [1] (1) | -304 [1] (2) | 166 [0] (1) |
| O(61,81) | 254 [0] (1) | -195 [0] (2) | 330 [0] (1) |
| O(62,83) | 396 [0] (1) | -136 [1] (2) | 322 [1] (1) |
| O(63,82) | 354 [1] (1) | -384 [2] (2) | 315 [2] (1) |
| O(64,84) | 348 [0] (1) | -248 [0] (2) | 434 [0] (1) |
| OW(1,2)  | 5 [1] (2)   | -287 [2] (3) | 0 [2] (2)   |
| OW(3,4)  | 222 [0] (2) | -42 [2] (2)  | 501 [2] (1) |

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## International Union of Crystallography

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The International Union of Crystallography announces the establishment of the Ewald Prize for outstanding contributions to the science of crystallography. The name of the prize has been chosen with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the Union's publication *Acta Crystallographica* from 1948 to 1959, and as the President of the Union from 1960 to 1963.

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