

Acta Cryst. (1990). C46, 728

Isotypism of the triclinic $Tl_8Mo_{10}O_{34}$ and $(NH_4)_8Mo_{10}O_{34}$ molybdates. By R. BENCHRIFA and R. DE PAPE,
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(Received 15 November 1989; accepted 28 November 1989)

Abstract

Although they were described in different cells, the two triclinic $P\bar{1}$ title compounds are strictly isotypic. The ammonium phase [Garin & Costamagna (1988). *Acta Cryst.* C44, 779–782] should be described with the standard axes chosen for $Tl_8Mo_{10}O_{34}$ ($a < b < c$; $\alpha, \beta, \gamma > 90^\circ$) [Touboul, Idoura & Toledano (1984). *Acta Cryst.* C40, 1652–1655]. The corresponding cell parameters of $(NH_4)_8Mo_{10}O_{34}$ obtained from the transformation matrix [100;001;–110] are close for the two cells (values for thallium phase are in italics): $a = 7.750$ (1), 7.703 (5); $b = 11.038$ (1), 10.703 (7); $c = 12.421$ (1), 12.216 (7) Å; $\alpha = 98.52$ (1), 97.68 (5); $\beta = 119.87$ (1), 118.76 (5); $\gamma = 99.18$ (1), 99.81 (5)°. The application of the transformation [Rot(110;00–1;010) + Tr(0; $\frac{1}{2}$;0)] to the coordinates of the NH_4 phase shows the similarity of the corresponding coordinates for the two phases.

The coordinates for $(NH_4)_8Mo_{10}O_{34}$ in standard axes and for $Tl_8Mo_{10}O_{34}$ are given in Table 1. All other relevant information is contained in the *Abstract*.

Table 1. Coordinates and equivalent isotropic thermal parameters for $(NH_4)_8Mo_{10}O_{34}$ in standard axes and of $Tl_8Mo_{10}O_{34}$

Standard deviation for the first phase recalculated from Garin & Costamagna (1988).

	x	y	z	$B_{eq}(\text{Å}^2)$
$(NH_4)_8Mo_{10}O_{34}$				
Mo(1)	0.0927 (3)	0.2459 (2)	0.1707 (2)	1.00
Mo(2)	0.4589 (3)	0.5765 (2)	0.2770 (2)	0.78
Mo(3)	0.2339 (3)	0.4758 (2)	0.4258 (2)	0.63
Mo(4)	0.6425 (3)	0.8097 (2)	0.5373 (2)	0.86
Mo(5)	–0.2275 (3)	–0.0481 (2)	0.1608 (2)	1.11
O(1)	0.109 (1)	0.299 (1)	0.360 (1)	1.17
O(2)	–0.058 (2)	0.074 (2)	0.140 (1)	1.58
O(3)	0.354 (1)	0.191 (1)	0.317 (1)	0.91
O(4)	0.290 (1)	0.421 (1)	0.272 (1)	1.04
O(5)	0.164 (2)	0.223 (1)	0.059 (1)	1.98
O(6)	–0.117 (2)	0.303 (1)	0.101 (2)	1.49

Table 1 (cont.)

	x	y	z	$B_{eq}(\text{Å}^2)$
O(7)	0.474 (1)	0.608 (1)	0.461 (1)	0.74
O(8)	0.527 (2)	0.511 (1)	0.171 (1)	1.21
O(9)	0.254 (2)	0.631 (1)	0.181 (1)	1.89
O(10)	0.284 (1)	0.509 (1)	0.583 (1)	1.07
O(11)	0.659 (1)	0.728 (1)	0.383 (1)	1.20
O(12)	0.039 (1)	0.541 (1)	0.345 (1)	1.76
O(13)	0.844 (2)	0.939 (1)	0.584 (2)	1.54
O(14)	0.421 (1)	0.853 (1)	0.445 (2)	1.66
O(15)	–0.111 (2)	–0.167 (2)	0.210 (1)	2.27
O(16)	–0.303 (3)	0.018 (2)	0.264 (2)	2.51
O(17)	–0.450 (2)	–0.121 (1)	0.016 (2)	1.99
N(1)	0.358 (3)	0.724 (2)	0.768 (2)	2.04
N(2)	0.293 (3)	0.908 (2)	0.199 (2)	2.91
N(3)	0.078 (3)	0.825 (2)	0.475 (2)	1.81
N(4)	0.179 (3)	0.422 (2)	0.091 (2)	1.67
$Tl_8Mo_{10}O_{34}$				
Mo(2)	0.1064 (3)	0.2390 (2)	0.1731 (2)	1.21
Mo(4)	0.4802 (3)	0.5753 (2)	0.2750 (2)	1.12
Mo(3)	0.2380 (3)	0.4773 (2)	0.4244 (2)	1.04
Mo(5)	0.6521 (3)	0.8184 (2)	0.5259 (2)	1.23
Mo(1)	–0.2237 (3)	–0.0651 (2)	0.1731 (2)	1.57
O(8)	0.119 (2)	0.297 (1)	0.367 (2)	1.2
O(4)	–0.058 (3)	0.070 (1)	0.150 (2)	2.2
O(7)	0.357 (3)	0.177 (1)	0.327 (2)	1.8
O(9)	0.305 (2)	0.416 (1)	0.276 (2)	1.5
O(6)	0.185 (3)	0.213 (2)	0.072 (2)	2.7
O(5)	–0.095 (3)	0.307 (2)	0.103 (2)	2.3
O(12)	0.484 (2)	0.609 (1)	0.459 (2)	1.3
O(14)	0.549 (3)	0.506 (1)	0.167 (2)	1.9
O(13)	0.284 (3)	0.631 (2)	0.183 (2)	2.9
O(11)	0.273 (2)	0.516 (1)	0.577 (2)	1.6
O(15)	0.680 (2)	0.728 (1)	0.375 (2)	1.6
O(10)	0.046 (3)	0.543 (2)	0.330 (2)	2.7
O(17)	0.862 (2)	0.952 (1)	0.578 (2)	1.6
O(16)	0.434 (3)	0.863 (2)	0.427 (2)	2.4
O(1)	–0.099 (3)	–0.187 (2)	0.221 (2)	2.3
O(3)	–0.299 (3)	–0.002 (2)	0.279 (2)	2.6
O(2)	–0.455 (3)	–0.135 (2)	0.027 (2)	2.9
Tl(3)	0.3549 (2)	0.7320 (1)	0.7801 (1)	2.32
Tl(4)	0.2896 (2)	0.9071 (1)	0.1832 (1)	2.73
Tl(1)	0.0986 (2)	0.8151 (1)	0.4752 (1)	2.02
Tl(2)	0.1653 (1)	0.4281 (1)	0.9163 (1)	2.24

References

- GARIN, J. L. & COSTAMAGNA. (1988). *Acta Cryst.* C44, 779–782.
TOUBOUL, M., IDOURA, C. & TOLEDANO, P. (1984). *Acta Cryst.* C40, 1652–1655.

0108-2701/90/040728-01\$03.00

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