Table 33A-4-001. TlH_2PO_4 (TDP). Fractional coordinates of atoms at RT [81Nel2].

Atom	Site symmetry	x	y	z
Tl	1	0.1279(3)	−0.0019(9)	0.2578(6)
P	1	0.1244(4)	0.5214(12)	0.7595(8)
O(1)	1	0.0736(5)	0.3956(17)	0.9472(11)
O(2)	1	0.0533(5)	0.6571(13)	0.6060(10)
O(3)	1	0.1908(4)	0.7696(12)	0.8293(9)
O(4)	1	0.1816(4)	0.2715(11)	0.6671(9)
H(1)	$\bar{1}$	0	0.5	0
H(2)	$\bar{1}$	0	0.5	0.5
H(3)	1	0.1849(7)	0.0006(29)	0.7577(17)

Table 33A-4-002. TlH_2PO_4 (TDP). Anisotropic temperature parameters of atoms at RT [81Nel2]. U_{ij} [$\cdot 10^{-2}$ Å^2] is defined by Eq. (d) in Introduction.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{31}	U_{12}
Tl	4.3(2)	3.8(2)	4.6(2)	0.7(2)	0.0(1)	0.0(2)
P	2.8(3)	2.1(2)	3.1(3)	0.2(2)	−0.1(2)	−0.2(2)
O(1)	4.2(4)	6.6(4)	5.8(4)	3.4(3)	2.1(3)	1.9(3)
O(2)	5.2(4)	3.4(3)	5.1(3)	1.5(3)	−2.1(3)	−0.8(3)
O(3)	4.7(3)	2.4(3)	5.0(3)	−0.3(3)	−1.4(2)	0.2(2)
O(4)	4.7(3)	2.3(2)	4.1(3)	−0.2(2)	0.8(2)	0.0(2)
H(1)	10.2(17)	6.2(10)	5.5(9)	1.6(8)	−1.1(10)	−2.7(11)
H(2)	8.3(12)	6.4(10)	7.2(11)	2.8(10)	3.0(10)	2.6(11)
H(3)	3.6(5)	7.0(8)	5.7(6)	−1.6(6)	0.2(4)	−1.2(5)

Table 33A-4-003. TlH_2PO_4 (TDP). Fractional coordinates in phase I [94Mat]. T = 373 K.

	x	y	z
Tl	0.1283(1)	0	0.25
P	0.3752(6)	0	0.25
O(1)	0.4332(18)	0.1352(63)	0.0753(45)
O(2)	0.3148(15)	0.2452(42)	0.3410(35)

Table 33A-4-004. TlH_2PO_4 (TDP). Anisotropic temperature parameters in phase I [94Mat]. T = 373 K. U_{ij} [$\cdot 10^{-3}$ Å^2] is defined by Eq. (d) in Introduction.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tl	49(1)	46(1)	44(1)	0	0	–19(1)
P	40(4)	34(3)	32(3)	0	0	6(5)
O(1)	74(15)	60(14)	65(16)	7(14)	35(15)	2(14)
O(2)	55(12)	38(10)	36(10)	0(9)	18(10)	4(8)

Table 33A-4-005. TlH_2PO_4 (TDP). Fractional coordinates and anisotropic temperature parameters at RT [79Odd]. Isotropic temperature parameter B is defined by Eq. (e) in Introduction.

	x	y	z	B [Å^2]
Tl	0.12848(2)	–0.00201(10)	0.25895(5)	2.16
P	0.3756(1)	–0.0033(6)	0.2395(3)	1.28
O(1)	0.4200(8)	–0.0833(22)	0.0390(18)	4.05
O(2)	0.4501(8)	0.1621(22)	0.3909(16)	3.35
O(3)	0.3121(7)	0.2769(16)	0.1723(12)	2.75
O(4)	0.3184(6)	–0.2335(20)	0.3312(12)	3.49

Table 33A-4-006. TlH_2PO_4 (TDP). Distances and angles for three different hydrogen bonds [81Nel2].

O(1)–H(1)–O(1′) and O(2)–H(2)–O(2′)		O(3)–H(3)–O(4′)	
Distances: [Å]			
O(1)–O(1′)	2.43(1)	O(3)–O(4′)	2.50(1)
O(2)–O(2′)	2.47(1)	O(3)–H(3)	1.15(2)
		H(3)–O(4′)	1.36(2)
Angle: [°]		O(3)–H(3)–O(4′)	177(1)

Table 33A-4-007. TlH_2PO_4 (TDP). Interatomic distances [Å] and bond angles [°] in phase I [94 Mat]. T = 373 K. The symmetry codes α and β refer to $\bar{x}$, $\bar{y}$, $\bar{z}$, and x, $\bar{y}$, 1/2 + $\bar{z}$, respectively.

P–O(1)	1.54(3)
P–O(2)	1.53(2)
O(1)–O(1$^{\alpha}$)	2.48(4)
O(2)–O(2$^{\beta}$)	2.59(3)
O(1)–P–O(1$^{\beta}$)	114(2)
O(1)–P–O(2)	108(1)
O(2)–P–O(2$^{\beta}$)	111(1)

Table 33A-4-008. TlH_2PO_4 (TDP). Interatomic distances [Å] and bond angles [°] of PO_4 at RT [79Odd].

P–O(1)	1.500(18)
P–O(2)	1.600(18)
P–O(3)	1.597(14)
P–O(4)	1.449(18)
mean	1.537(17)
O(1)–P–O(2)	110.5(11)
O(1)–P–O(3)	101.6(9)
O(1)–P–O(4)	116.0(10)
O(2)–P–O(3)	99.2(9)
O(2)–P–O(4)	116.6(10)
O(3)–P–O(4)	110.6(9)
mean	109.1(10)