

Table 33A-10-001. TiH₂AsO₄ (TDA). Unit cell parameters at 293 K and 395 K [94Iro].

a [Å]	b [Å]	c [Å]	β [°]
14.515(3)	4.635(1)	6.610(5)	92.43(3) (293 K)
14.591(5)	4.647(2)	6.641(2)	(395 K)

Table 33A-10-002. TiD₂AsO₄ (DTDA). Fractional coordinates and isotropic temperature parameters of atoms [87Nar1]. The isotropic temperature parameter U_{eq} is defined as $U_{\text{eq}} = (U_{11} + U_{22} + U_{33})/3$, where U_{ii} are defined by Eq. (d) in Introduction. Deuteration rate: 80(5)%.
(d) in Introduction.

	x	y	z	U_{eq} [Å ²]
Ti	0.2646(3)	0.0103(9)	0.1240(1)	0.0466(6)
As	0.7630(6)	0.4929(21)	0.1289(3)	0.0360(11)
O(1)	0.9611(44)	0.3964(71)	0.0727(24)	0.0705(15)
O(2)	0.5927(37)	0.6681(57)	0.0480(21)	0.0381(11)
O(3)	0.6517(40)	0.2492(40)	0.1896(19)	0.0399(11)
O(4)	0.8388(45)	0.7885(83)	0.2010(22)	0.0579(14)

Table 33A-10-003. TiD₂AsO₄ (DTDA). Interatomic distances [Å] and angles [°] [87Nar1].

As–O(2)	1.766(28) Å	O(1)–As–O(4)	108.5(15)°
As–O(1)	1.658(22)	O(2)–As–O(3)	111.8(13)
As–O(3)	1.680(29)	O(2)–As–O(4)	104.2(15)
As–O(4)	1.741(36)	O(3)–As–O(4)	109.9(15)
O(1)–O(1 ⁱ)	2.403(58)	O(1)–As–O(3)	114.4(16)
O(2)–O(2 ⁱⁱ)	2.403(48)	O(2)–As–O(1)	107.5(15)
O(3)–O(4 ⁱⁱⁱ)	2.479(48)		

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $-1-x, 1-y, -z$; (iii) $x, y-1, z$.