

**Table 35A-7-001.** KVOPO<sub>4</sub>. Atomic coordinates and temperature parameters [90Phi].

$$U_{\text{eq}} = \frac{1}{3}(U_{11} + U_{22} + U_{33}).$$

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>eq</sub> [Å <sup>2</sup> ]
K(1)	0.3819(2)	0.7815(4)	0.3173(3)	0.0245
K(2)	0.1032(2)	0.7056(4)	0.0701(3)	0.0242
V(1)	0.3761(1)	0.4967(2)	0.0003(2)	0.0105
V(2)	0.2486(1)	0.2734(2)	0.2520(2)	0.0101
P(1)	0.4978(2)	0.3308(3)	0.2614(3)	0.0093
P(2)	0.1805(1)	0.4985(4)	0.5155(3)	0.0085
O(1)	0.4835(6)	0.477(1)	0.1486(6)	0.0127
O(2)	0.5100(6)	0.473(1)	0.3821(6)	0.0153
O(3)	0.3988(5)	0.196(1)	0.2842(7)	0.0109
O(4)	0.5941(5)	0.188(1)	0.2451(7)	0.0100
O(5)	0.1113(5)	0.306(1)	0.5450(6)	0.0125
O(6)	0.1102(5)	0.688(1)	0.4866(7)	0.0105
O(7)	0.2534(6)	0.538(1)	0.6326(6)	0.0133
O(8)	0.2558(6)	0.454(1)	0.4049(6)	0.0129
O(9)	0.2726(6)	0.463(1)	0.1471(6)	0.0138
O(10)	0.2212(6)	0.032(1)	0.3969(7)	0.0150

**Table 35A-7-002.** KVOPO<sub>4</sub>. Bond distances and angles [90Phi].

Distances [Å]			
V(1)–O(1)	2.089(7)	K(1)–O(1)	2.943(8)
V(1)–O(2)	1.930(7)	K(1)–O(2)	2.653(9)
V(1)–O(5)	2.040(7)	K(1)–O(3)	2.679(7)
V(1)–O(6)	1.986(7)	K(1)–O(5)	2.880(7)
V(1)–O(9)	2.051(7)	K(1)–O(7)	3.081(8)
V(1)–O(10)	1.673(8)	K(1)–O(8)	2.800(8)
		K(1)–O(9)	3.053(8)
V(2)–O(3)	2.016(7)	K(1)–O(10)	2.741(8)
V(2)–O(4)	1.997(6)		
V(2)–O(7)	1.962(7)	K(2)–O(1)	2.675(8)
V(2)–O(8)	1.987(7)	K(2)–O(2)	2.995(9)
V(2)–O(9)	1.671(8)	K(2)–O(3)	3.019(8)
V(2)–O(10)	2.199(8)	K(2)–O(4)	3.123(7)
		K(2)–O(5)	2.764(7)
P(1)–O(1)	1.524(8)	K(2)–O(7)	2.884(8)
P(1)–O(2)	1.574(8)	K(2)–O(8)	2.971(8)
P(1)–O(3)	1.553(7)	K(2)–O(9)	2.787(8)
P(1)–O(4)	1.543(6)	K(2)–O(10)	3.104(8)
P(2)–O(5)	1.545(7)		
P(2)–O(6)	1.540(7)		
P(2)–O(7)	1.570(7)		
P(2)–O(8)	1.541(8)		
Angles [deg]			
V(1)–O(9)–V(2)	134.0(4)	V(1)–O(10)–V(2)	131.9(4)
O(10)–V(1)–O(9)	91.4(3)	O(10)–V(2)–O(9)	177.2(4)