

**Table 35A-13-001.** TiTiOPO<sub>4</sub>. Raman shifts of several modes [90Pis].  $T = 110$  K. Corresponding geometries:  $Y(XY)X$ ,  $Y(ZX)\bar{Y}$ ,  $X(ZY)\bar{X}$ ,  $Y(ZZ)X$  and  $Z(YY)\bar{Z}$  from left hand column. The shifts with asterisks were measured in  $X(YY)\bar{X}$  geometry.

$\Delta\nu [\text{cm}^{-1}]$				
$A_2$	$B_1$ (transverse)	$B_2$ (transverse)	$A_1$ (transverse)	$A_1$ (longitudinal)
28.8	26	27.3	30.7	31.0
31.0	30.4	37.7	41.3	41.7
39.7	(37.7)	52.7	43.9	44.7
45.7	51.9	69.2	44.9*	(51.9)
(52.5)	61.2	(89.0)	52.5	54.3
56.7	(69.9)	98.0	61.5	62.3
65.5	76.0	109.0	70.4	70.6
(70.4)	(89.0)	(129.2)	92.1	92.6
76.7	98.3	137.7	129.3	129.3
90.3	(129.2)	156.1	155.5	156.5
98.5	136.7	(164.5)	161.3	151.7
(129.2)	177.5	166.5	202.0	202.4
131.8	183.2	202.0	203.6	(207.5)
136.4	(203.6)	214.9	232.7	232.8
153.0	204.7	220.1	238.6	238.8
164.5	207.5	225.5	259.0	
192.8	(228.5)	(228.5)	265.9	(266.2)
(228.5)	(234.6)	234.4	274.5	
234.6	244.6	238.6	289.8	289.8
250.6	252.9	263.6	303.6	
286.4	270.0	282.7	314.9*	(317.0)
294.1	288.3	302.0	334.3	(337.5)
315.6	295.3	316.7	(335.7)*	
336.3	309.5	327.6	361.6	361.8
(403.8)	311.6	(341.0)	373.3*	
410.4	335.7	362.6	388.5	388.6
472.8	397.2	374.4	415.6	
500.4	408.0	383.9	469.0*	(482.0)
516.0	416.9	403.8	515.2	516.3
536.3	471.7	409.1	544.6*	545.6
567.2	481.1	472.5	567.9*	568.1
588.0	492.1	552.1	580.0	582.2
(656.1)	557.5	561.2	588.6	588.8
774.4	586.3	587.0	613.0	614.5
800.2	614.6	616.7	654.1	736.3
818.9	(656.1)	(656.1)	818.0	818.3
956.7	699.3	817.3	935.0	
1013.7	766.4	959.4	962.3	962.6
1029.0	796.9	980.6	983.7	984.2
1064.7	(818.9)	996.5	987.8	987.8
1074.4	960.4	999.6	998.8*	1000.3
1102.0	984.8	1022.7	1013.3*	(1020.5)
	995.1	(1075.3)	1025.3	
	1023.8	1079.9	1074.9	(1074.9)
	1075.7	1106.2		