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ARTICLE TYPE

$H_2Ti_6O_{13}$, a new protonated titanate prepared by Li^+/H^+ ion exchange: synthesis, crystal structure and electrochemical Li insertion properties

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Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX

DOI: 10.1039/b000000x

Supplementary Information

Table I Refined lattice parameters of $Li_2Ti_6O_{13}$ and $H_2Ti_6O_{13}$ obtained by Rietveld analysis of XRD data. Reliability factors are also included

	Space Group	*a* (Å)	*b* (Å)	c (Å)	β (º)	χ^2	R_{wp}	R_{exp}	R_B
$Li_2Ti_6O_{13}$	C2/m	15.3457(7)	3.7527(1)	9.1528(2)	99.466(2)	2.21	5.74	3.87	7.50
$H_2Ti_6O_{13}$	C2/m	14.6731(3)	3.7461(1)	9.2641(2)	96.934(1)	1.48	4.77	3.92	4.87

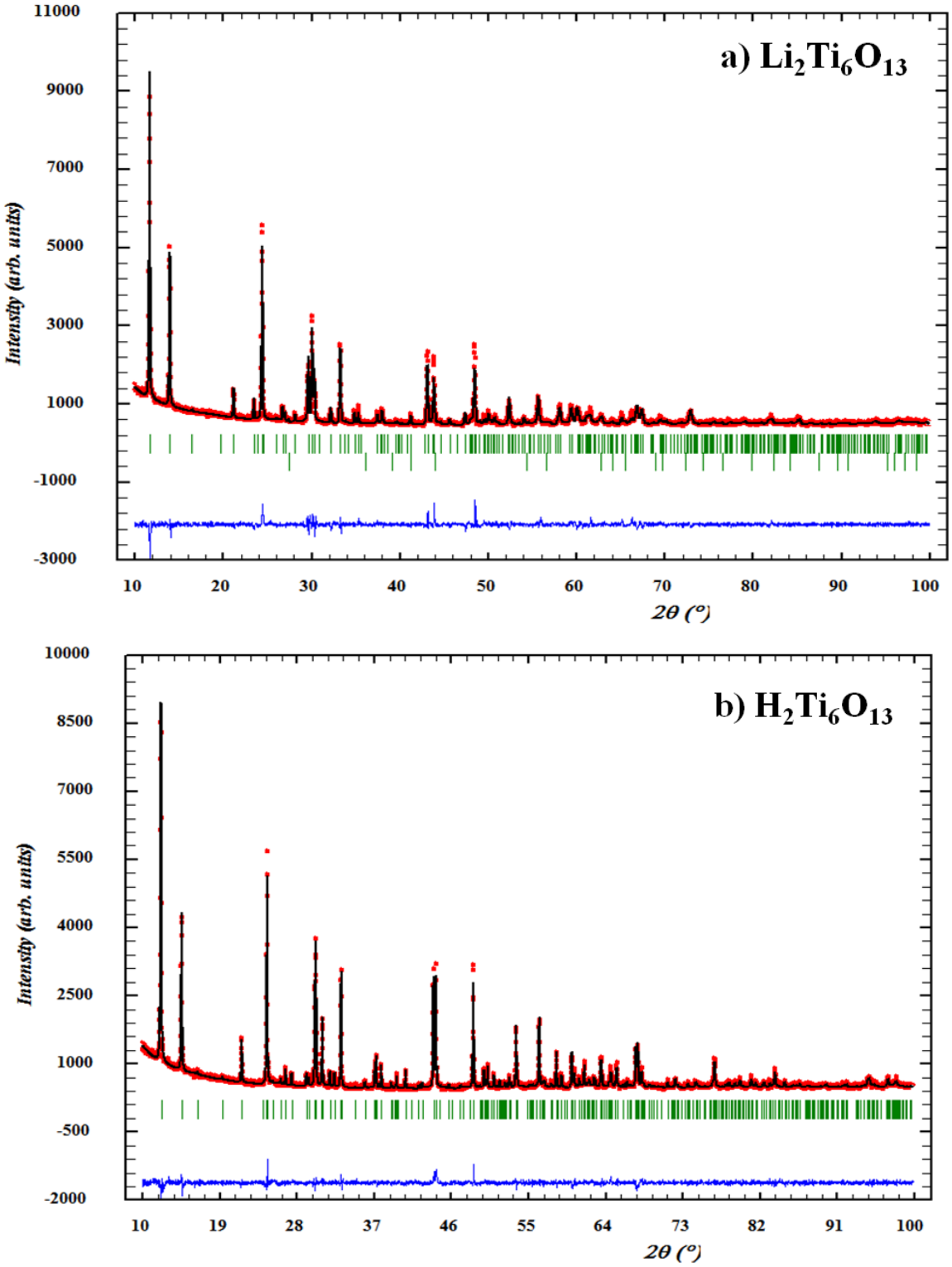

Fig. 1 Experimental (red circles) and calculated (black continuous line) XRD patterns (and their difference, blue line at the bottom) for a) $Li_2Ti_6O_{13}$ and b) $H_2Ti_6O_{13}$. For the former the intensities of Bragg peaks corresponding to TiO_2 as a second row of vertical green bars are also shown

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Table II Refined lattice parameters and reliability factor for $Li_2Ti_6O_{13}$ and $H_2Ti_6O_{13}$ obtained by Rietveld analysis of synchrotron diffraction data

	$Li_2Ti_6O_{13}$	$H_2Ti_6O_{13}$
Space Group	C2/m	C2/m
***a* (Å)**	15.2780(12)	14.5964(14)
***b* (Å)**	3.7333(3)	3.7283(4)
***c* (Å)**	9.0962(8)	9.2162(8)
β (º)	99.495(4)	96.929(4)
V (Å^3)	511.71(7)	497.86(8)
χ^2	1.82	5.21
R_{wp}	2.88	4.12
R_{exp}	2.14	1.81
R_B	3.46	2.49

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Table III Structural parameters of $Li_2Ti_6O_{13}$ and $H_2Ti_6O_{13}$ obtained by Rietveld analysis of synchrotron diffraction data

$Li_2Ti_6O_{13}$						
Atom	**Site**	**x**	**y**	**z**	**B (Å^2)**	**Occupancy**
Ti1	4i	0.11608(28)	0	0.09567(49)	0.625(92)	1
Ti2	4i	0.16843(37)	0	0.43823(56)	1.360(96)	1
Ti3	4i	0.23109(27)	0	0.76982(46)	0.418(81)	1
O1	2a	0	0	0	0.105(73)	0.5
O2	4i	0.24197(81)	0	0.24643(148)	0.105(73)	1
O3	4i	0.07186(85)	0	0.28919(135)	0.105(73)	1
O4	4i	0.29839(91)	0	0.56431(164)	0.105(73)	1
O5	4i	0.13090(85)	0	0.61041(135)	0.105(73)	1
O6	4i	0.35428(73)	0	0.89615(135)	0.105(73)	1
O7	4i	0.16028(77)	0	0.91134(153)	0.105(73)	1
$H_2Ti_6O_{13}$						
Atom	**Site**	**x**	**y**	**z**	**B (Å^2)**	**Occupancy**
Ti1	4i	0.11410(41)	0	0.09205(54)	2.617(195)	1
Ti2	4i	0.16270(50)	0	0.44923(58)	0.206(136)	1
Ti3	4i	0.22770(47)	0	0.77191(56)	0.987(156)	1
*O1	2a	0	0	0	0.105	0.5
*O2	4i	0.23992(62)	0	0.25210(75)	0.105	1
*O3	4i	0.06058(68)	0	0.28828(75)	0.105	1
*O4	4i	0.30139(63)	0	0.55798(84)	0.105	1
*O5	4i	0.12274(50)	0	0.61923(73)	0.105	1
*O6	4i	0.35418(49)	0	0.88590(78)	0.105	1
*O7	4i	0.16844(76)	0	0.91976(90)	0.105	1