Refinement of the crystal structure of lithium nickel phosphate, $LiNiPO_4$

S. A. Warda and S.-L. Lee

Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str., D-35032 Marburg, Germany

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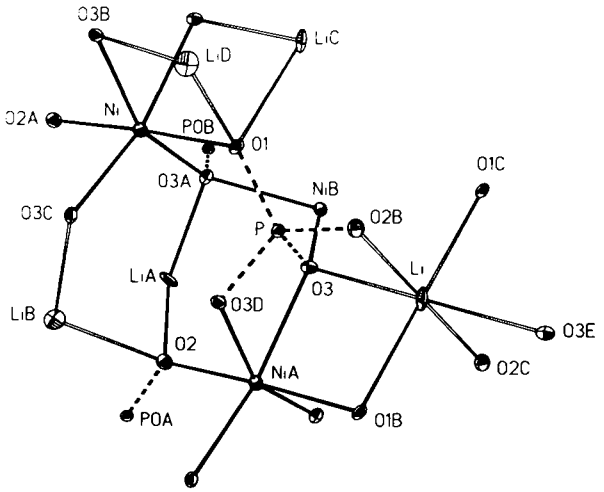

Source of material: The compound was synthesized from $NiNH_4PO_4$ and Li_3PO_4, the crystals were grown from a melt of Li_2SO_4 (see ref. 2).

We succeded in obtaining crystals of $LiNiPO_4$ suitable for single crystal structural analysis. The data resulting from the structural determination are in agreement with the parameters reported previously from powder diffraction data on the same compound (see ref. 1). The tetrahedral coordination spheres of the oxygen atoms typical for olivine structures are of great interest for our theoretical calculations. While O1 and O2 are coordinated by one P, two Li and one Ni, the O3 is surrounded by one P, one Li and two Ni (see figure).

Table 1. Parameters used for the X-ray data collection

Crystal:	brown prism, size 0.10 x 0.13 x 0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	74.38 cm^{-1}
Diffractometer:	Enraf Nonius CAD4
Scan mode:	ω
$T_{measurement}$:	293 K
$2\theta_{max}$:	52.5°
$N(hkl)_{unique}$:	307
Criterion for I_o:	$I_o > 2\,\sigma(I_o)$
$N(param)_{refined}$:	41
Programs:	SHELXS-96, SHELXL-96, SHELXTL-96

$LiNiO_4P$, orthorhombic, *Pnma* (No. 62), a =10.032(1) Å, b =5.855(1) Å, c =4.681(1) Å, V =274.9 $Å^3$, Z =4, $R(F)$ =0.036, $R_w(F^2)$ =0.096.

Table 2. Final atomic coordinates and displacement parameters (in $Å^2$)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Li	4*a*	0	0	0	0.011(4)	0.009(5)	0.012(4)	−0.004(4)	−0.004(3)	−0.004(3)
Ni	4*c*	0.27563(6)	1/4	0.9828(1)	0.0048(7)	0.0056(6)	0.0065(6)	0	0.0000(2)	0
P	4*c*	0.0944(1)	1/4	0.4177(3)	0.0047(8)	0.0052(8)	0.0042(8)	0	−0.0005(5)	0
O(1)	4*c*	0.0998(3)	1/4	0.7422(8)	0.006(2)	0.009(2)	0.004(2)	0	−0.002(1)	0
O(2)	4*c*	0.4517(3)	1/4	0.2011(8)	0.007(2)	0.008(2)	0.008(2)	0	0.001(1)	0
O(3)	8*d*	0.1659(2)	0.0426(4)	0.2779(5)	0.008(1)	0.005(1)	0.006(1)	0.0011(8)	0.0018(8)	0.000(1)

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