

Table 1 Quantum-optimized structural parameters at 0 K for the structure of LiNaSiB₃O₇(OH)

Atom	x	y	z
Li	0.46056	0.19786	0.13025
Na	0.96068	0.99327	0.75540
Si	0.04065	0.75195	0.20939
B(1)	0.23254	0.14853	0.68134
B(2)	0.68153	0.35379	0.41433
B(3)	0.53467	0.50064	0.79253
O(1)	0.80482	0.72223	0.97854
O(2)	0.27333	0.78588	0.20991
O(3)	0.97384	0.84843	0.29786
O(4)	0.11932	0.64582	0.35918
O(5)	0.75115	0.54799	0.88873
O(6)	0.68271	0.45875	0.34996
O(7)	0.54386	0.66866	0.61572
O(8)	0.54383	0.40331	0.84823
H(1)	0.69726	0.30846	0.96131

P2₁/c, a = 6.69305 Å, b = 13.65570 Å, c = 7.54886 Å, β = 123.858°

Table 2 Final refined structural parameters of LiNaSiB₃O₇(OH)

Atom	x	y	z	U _{iso} (Å ³)
Li	0.4623(20)	0.1995(6)	0.1383(15)	0.046(3)
Na	0.9733(3)	0.9906(1)	0.7544(3)	aniso
Si	0.0378(4)	0.7539(2)	0.2048(3)	0.0548(5)
B(1)	0.2096(17)	0.1602(8)	0.6623(18)	0.092(3)
B(2)	0.6920(14)	0.3493(6)	0.4160(15)	0.054(3)
B(3)	0.5290(10)	0.5022(4)	0.7860(9)	aniso
O(1)	0.8157(7)	0.7241(3)	0.9895(6)	0.065(1)
O(2)	0.2673(7)	0.7818(3)	0.2102(6)	0.066(1)
O(3)	0.9733(6)	0.8484(3)	0.2873(7)	0.058(1)
O(4)	0.1150(6)	0.6584(3)	0.3491(6)	0.054(1)
O(5)	0.7457(8)	0.5506(3)	0.8761(9)	0.071(2)
O(6)	0.6846(9)	0.4560(3)	0.3520(8)	0.057(1)
O(7)	0.5489(7)	0.6725(3)	0.6198(6)	0.063(1)
O(8)	0.5299(3)	0.4051(3)	0.8362(6)	0.073(1)
H(1)	0.6992(3)	0.3993(14)	0.9359(30)	0.095(2)

P2₁/c, a = 6.7620(1) Å, b = 13.8016(3) Å, c = 7.6878(2) Å, β = 124.0894(9)°, volume = 594.18(2) Å³

R_{wp} = 4.2%, R_{wp'} = 7.0%, R_p = 2.9%, R_{p'} = 5.6%, GOF(Rietveld) = 2.7, GOF(R_{wp}(Rietveld)/R_{wp}(Pawley)) = 1.27, DW = 1.76, R_B = 1.3%

Na (U₁₁ = 0.091(6), U₂₂ = 0.066(2), U₃₃ = 0.081(2), U₁₂ = 0.010(7), U₁₃ = 0.038(2), U₂₃ = -0.005(2))

B(3) (U₁₁ = 0.046(7), U₂₂ = 0.158(9), U₃₃ = 0.098(11), U₁₂ = 0.016(7), U₁₃ = 0.043(8), U₂₃ = 0.078(8))