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$(Na,Li)_3(Cl,OH)[Cu_3OAl(PO_4)_3]$: a first salt-inclusion aluminophosphate oxocuprate with the original crystal structure

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Table S1 Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.250000	0.250000	0.500000	0.0109 (2)	
Cu2	0.12705 (5)	0.41671 (3)	0.31049 (7)	0.01122 (16)	
Cu3	0.000000	0.24835 (5)	0.500000	0.0138 (2)	
Cu4	0.62554 (8)	0.74519 (3)	0.82896 (7)	0.02009 (19)	
P1	0.12573 (12)	0.26303 (7)	0.19526 (14)	0.0112 (3)	
P2	0.11905 (10)	0.61919 (6)	0.66727 (13)	0.0068 (2)	
P3	0.63242 (10)	0.61716 (7)	0.65454 (13)	0.0080 (3)	
Al1	0.24664 (16)	0.500000	0.5261 (2)	0.0073 (4)	
Al2	0.000000	0.500000	0.500000	0.0060 (6)	
Al3	0.500000	0.500000	0.500000	0.0086 (6)	
Na1	0.000000	0.60798 (18)	1.000000	0.0116 (6)	
Na2	0.74974 (18)	0.61404 (16)	1.0123 (3)	0.0231 (6)	
Na3	0.6188 (3)	0.6185 (2)	0.3120 (4)	0.0129 (12)	0.556 (10)
Li1	0.6222 (17)	0.5757 (14)	0.300 (2)	0.0129 (12)	0.444 (10)
Na4	0.504 (2)	0.6190 (6)	1.0348 (16)	0.064 (6)	0.420 (15)
Li2	0.504 (2)	0.6190 (6)	1.0348 (16)	0.064 (6)	0.080 (15)
Cl2	0.6191 (3)	0.5102 (4)	1.0679 (3)	0.0147 (17)	0.375 (4)
O15	0.5411 (17)	0.500000	0.847 (2)	0.0147 (17)	0.251 (8)
Cl1	0.13134 (16)	0.500000	0.06802 (19)	0.0146 (4)	

O1	0.3752 (4)	0.500000	0.5926 (5)	0.0088 (9)	
O2	0.1252 (4)	0.500000	0.4326 (5)	0.0064 (9)	
O3	0.2119 (3)	0.5716 (2)	0.6616 (4)	0.0113 (7)	
O4	0.7272 (3)	0.5722 (2)	0.6287 (4)	0.0114 (8)	
O5	0.0234 (3)	0.5724 (2)	0.6514 (4)	0.0082 (7)	
O6	0.1167 (3)	0.65488 (18)	0.8223 (4)	0.0084 (7)	
O7	0.6308 (3)	0.6793 (2)	0.5442 (4)	0.0182 (8)	
O8	0.1191 (3)	0.6728 (2)	0.5402 (4)	0.0156 (8)	
O9	0.5405 (3)	0.5711 (2)	0.6362 (4)	0.0136 (8)	
O10	0.6358 (3)	0.64578 (18)	0.8147 (4)	0.0097 (7)	
O11	0.2212 (3)	0.2434 (2)	0.2855 (5)	0.0147 (8)	
O12	0.0305 (3)	0.2412 (2)	0.2816 (5)	0.0185 (9)	
O13	0.1248 (3)	0.34339 (19)	0.1676 (4)	0.0102 (7)	
O14	0.1273 (5)	0.2248 (2)	0.0484 (5)	0.0360 (12)	