

# Na-Alternative to Tinsleyite Obtained under Hydrothermal Conditions: Crystal Structure and Comparative Crystal Chemistry

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**Table S1.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for  $\text{Na}_2\text{Al}_2\text{O}(\text{PO}_4)_2 \cdot 0.12\text{H}_2\text{O}$ .

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> <sub>iso</sub> <sup>*</sup> / <i>U</i> <sub>eq</sub>	Occ. (< 1)
P1	−0.09688 (4)	0.88033 (4)	0.64790 (4)	0.00531 (8)	
P2	0.36894 (4)	0.62263 (4)	0.60107 (4)	0.00562 (8)	
Al1	0.11711 (5)	0.40130 (5)	0.55369 (5)	0.00530 (9)	
Al2	0.18162 (5)	0.68842 (5)	0.78063 (5)	0.00545 (9)	
Na1	0.77484 (14)	0.5582 (3)	0.7802 (2)	0.0132 (4)	0.930 (12)
Na1'	0.7612 (19)	0.523 (3)	0.807 (3)	0.0132 (4)	0.070 (12)
Na2	0.45030 (7)	0.28310 (8)	0.56427 (8)	0.01594 (14)	
O1	−0.06181 (11)	0.41235 (11)	0.39508 (11)	0.00654 (19)	
O2	−0.14023 (12)	1.04509 (12)	0.60626 (11)	0.0081 (2)	
O3	0.07392 (12)	0.86257 (12)	0.72444 (12)	0.00759 (19)	
O4	−0.16734 (12)	0.78916 (12)	0.49913 (11)	0.00739 (19)	
O5	−0.15697 (12)	0.81896 (12)	0.75910 (12)	0.0076 (2)	
O6	0.31578 (12)	0.72787 (12)	0.46346 (12)	0.0093 (2)	
O7	0.33626 (12)	0.69011 (13)	0.73005 (12)	0.0112 (2)	
O8	0.53386 (12)	0.59611 (13)	0.66082 (13)	0.0125 (2)	
O9	0.28443 (12)	0.47053 (12)	0.54952 (13)	0.0094 (2)	
O10	0.500000	0.000000	0.500000	0.081 (14)	0.121 (11)