

## SUPPORTING INFORMATION

### **Na<sub>3</sub>(VO)(PO<sub>4</sub>)(CO<sub>3</sub>): a synthetic member of the bradleyite phosphate carbonate family with a new type of crystal structure**

Olga Yakubovich,<sup>\*a</sup> Galina Kiriukhina,<sup>a,b</sup> Sergey Simonov,<sup>c</sup> Anatoly Volkov<sup>d</sup> and Olga Dimitrova<sup>a</sup>

<sup>a</sup> Lomonosov Moscow State University, Moscow, 119991, Russia.

<sup>b</sup> Korzhinskii Institute of Experimental Mineralogy RAS, Chernogolovka, Moscow region, 142432, Russia.

<sup>c</sup> Institute of Solid State Physics RAS, Chernogolovka, Moscow region, 142432, Russia.

<sup>d</sup> Skolkovo Institute of Science and Technology, Moscow, 121205, Russia.

E-mail: yakubovich.olga320@gmail.com

**Table S1.** Na<sub>3</sub>(VO)[PO<sub>4</sub>][CO<sub>3</sub>]. Atomic coordinates and equivalent isotropic displacement parameters (Å × 10<sup>3</sup>).  $U_{(eq)}$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

Atom	x/a	y/b	z/c	$U_{(eq)}$
V	0.47387(6)	0.25	0.22774(4)	0.00481(8)
P	0.54775(9)	0.25	-0.12178(6)	0.00559(11)
Na1	0.29437(15)	0.25	0.52688(10)	0.01133(18)
Na2	1.07052(11)	0.49294(14)	0.82776(7)	0.01190(14)
C	0.8254(3)	0.25	0.4824(2)	0.0064(4)
O1	0.6168(3)	0.25	0.47073(18)	0.0094(3)
O2	0.9833(3)	0.25	0.6156(2)	0.0091(3)
O3	0.4650(2)	0.0567(2)	-0.23280(12)	0.0090(2)
O4	0.8586(3)	0.25	0.3467(2)	0.0090(3)
O5	0.4129(3)	0.25	-0.0056(2)	0.0108(3)
O6	0.7990(3)	0.25	-0.0343(2)	0.0107(3)
O7	0.2237(3)	0.25	0.2351(2)	0.0092(3)