Supplementary Materials

Synthesis, Crystal Structure, and Nonlinear Optical Properties of a New Alkali and Alkaline Earth Metal Carbonate RbNa5Ca5(CO3)8

Qiaoling Chen and Min Luo

**Table S1.** Atomic coordinates and equivalent isotropic displacement parameters. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **atom** | **x** | **Y** | **z** | **Ueq(Å2)** | **BVS** | **Occ** |
| Rb(1) | 3333 | 6667 | 3892(1) | 35(1) | 0.96 | 1 |
| Ca(1) | 5054(1) | 10108(2) | 1167(1) | 15(1) | 2.01 | 1 |
| Ca(2) | 0 | 10000 | 531(2) | 11(1) | 2.07 | 1 |
| Na(1) | 1459(2) | 2918(3) | 2294(2) | 21(1) | 1.28 | 1 |
| Na(2) | 1841(1) | 8159(1) | −583(2) | 17(1) | 1.09 | 0.33 |
| Ca(3) | 1841(1) | 8159(1) | −583(2) | 17(1) | 1.80 | 0.67 |
| C(1) | −1664(4) | 11664(4) | 748(6) | 16(1) | 4.06 | 1 |
| C(2) | 3333 | 6667 | 1258(10) | 12(2) | 4.02 | 1 |
| C(3) | 5171(4) | 4829(4) | 3429(5) | 14(1) | 4.02 | 1 |
| C(4) | 0 | 10000 | 3317(9) | 12(3) | 4.01 | 1 |
| O(1) | 5400(3) | 4600(3) | 4401(4) | 24(1) | 2.01 | 1 |
| O(2) | 2600(3) | 7400(3) | 1278(5) | 24(1) | 2.16 | 1 |
| O(3) | 2387(3) | 7613(3) | 5778(5) | 23(1) | 2.03 | 1 |
| O(4) | −2395(4) | 10191(3) | 728(3) | 19(1) | 2.08 | 1 |
| O(5) | 3972(4) | 3832(5) | 2951(3) | 38(1) | 1.96 | 1 |
| O(6) | 0 | 10000 | 2304(7) | 32(2) | 1.92 | 1 |
| O(7) | 549(8) | 11099(16) | 3803(10) | 193(12) | 2.37 | 0.67 |

**Table S2.** Bond lengths (Å) for RbNa5Ca5(CO3)8.

|  |  |  |  |
| --- | --- | --- | --- |
| Rb(1)-O(3) | 2.900(6) | Na(2)-O(7)#13 | 2.960(5) |
| Rb(1)-O(3)#1 | 2.900(6) | Na(2)-O(7)#12 | 2.960(5) |
| Rb(1)-O(3)#2 | 2.900(6) | C(1)-O(3)#12 | 1.264(8) |
| Rb(1)-C(3)#1 | 3.261(7) | C(1)-O(4)#5 | 1.285(5) |
| Rb(1)-C(3)#2 | 3.261(7) | C(1)-O(4) | 1.285(5) |
| Rb(1)-C(3) | 3.261(7) | C(1)-Ca(1)#15 | 2.914(4) |
| Rb(1)-C(2) | 3.330(13) | C(1)-Ca(1)#21 | 2.914(4) |
| Rb(1)-O(5)#1 | 3.439(5) | C(1)-Rb(1)#12 | 3.740(7) |
| Rb(1)-O(5)#3 | 3.439(5) | C(2)-O(2) | 1.281(5) |
| Rb(1)-O(5)#4 | 3.439(5) | C(2)-O(2)#1 | 1.281(5) |
| Rb(1)-O(5)#2 | 3.439(5) | C(2)-O(2)#2 | 1.281(5) |
| Rb(1)-O(5)#5 | 3.439(5) | C(2)-Ca(1)#2 | 3.0051(17) |
| Ca(1)-O(1)#6 | 2.368(5) | C(2)-Ca(1)#1 | 3.0051(17) |
| Ca(1)-O(3)#7 | 2.4981(18) | C(3)-O(5) | 1.273(5) |
| Ca(1)-O(3)#8 | 2.4981(18) | C(3)-O(5)#5 | 1.273(5) |
| Ca(1)-O(5)#2 | 2.511(5) | C(3)-O(1) | 1.292(8) |

**Table 2.** *Cont.*

|  |  |  |  |
| --- | --- | --- | --- |
| Ca(1)-O(5)#4 | 2.511(5) | C(3)-Ca(1)#1 | 2.866(7) |
| Ca(1)-O(4)#9 | 2.590(4) | C(3)-Ca(3)#22 | 2.891(4) |
| Ca(1)-O(4)#10 | 2.590(4) | C(3)-Na(2)#22 | 2.891(4) |
| Ca(1)-O(2) | 2.6138(16) | C(3)-Ca(3)#23 | 2.891(4) |
| Ca(1)-O(2)#1 | 2.6138(16) | C(3)-Na(2)#23 | 2.891(4) |
| Ca(1)-C(3)#2 | 2.866(7) | C(4)-O(7)#11 | 1.138(15) |
| Ca(1)-C(1)#9 | 2.914(4) | C(4)-O(7) | 1.138(15) |
| Ca(1)-C(1)#11 | 2.914(4) | C(4)-O(7)#15 | 1.138(15) |
| Ca(2)-O(6) | 2.241(9) | C(4)-O(6) | 1.281(15) |
| Ca(2)-O(7)#12 | 2.385(13) | C(4)-Ca(2)#24 | 2.798(12) |
| Ca(2)-O(7)#8 | 2.385(13) | C(4)-Na(1)#25 | 2.856(6) |
| Ca(2)-O(7)#13 | 2.385(13) | C(4)-Na(1)#1 | 2.856(6) |
| Ca(2)-O(4)#11 | 2.527(4) | C(4)-Na(1)#26 | 2.856(6) |
| Ca(2)-O(4)#10 | 2.527(4) | O(1)-Ca(1)#23 | 2.368(5) |
| Ca(2)-O(4)#14 | 2.527(4) | O(1)-Ca(3)#22 | 2.432(3) |
| Ca(2)-O(4)#15 | 2.527(4) | O(1)-Na(2)#22 | 2.432(3) |
| Ca(2)-O(4) | 2.527(4) | O(1)-Ca(3)#23 | 2.432(2) |
| Ca(2)-O(4)#5 | 2.527(4) | O(1)-Na(2)#23 | 2.432(2) |
| Ca(2)-C(4)#12 | 2.798(12) | O(2)-Na(1)#1 | 2.369(6) |
| Ca(2)-C(1)#15 | 2.916(7) | O(2)-Ca(1)#2 | 2.6138(16) |
| Na(1)-O(2)#2 | 2.369(6) | O(3)-C(1)#24 | 1.264(8) |
| Na(1)-O(5) | 2.370(4) | O(3)-Ca(1)#27 | 2.4981(18) |
| Na(1)-O(5)#3 | 2.370(4) | O(3)-Ca(1)#28 | 2.4981(18) |
| Na(1)-O(4)#16 | 2.466(4) | O(4)-Ca(3)#11 | 2.443(4) |
| Na(1)-O(4)#17 | 2.466(4) | O(4)-Na(2)#11 | 2.443(4) |
| Na(1)-O(7)#18 | 2.481(13) | O(4)-Na(1)#25 | 2.466(4) |
| Na(1)-O(6)#18 | 2.546(3) | O(4)-Ca(1)#21 | 2.590(4) |
| Na(1)-C(4)#18 | 2.856(6) | O(5)-Ca(1)#1 | 2.511(5) |
| Na(1)-Ca(2)#18 | 3.384(3) | O(5)-Ca(3)#23 | 2.637(5) |
| Na(1)-Ca(1)#1 | 3.453(2) | O(5)-Na(2)#23 | 2.637(5) |
| Na(1)-Ca(1)#2 | 3.453(2) | O(6)-Na(1)#1 | 2.546(3) |
| Na(1)-Na(2)#2 | 3.698(4) | O(6)-Na(1)#26 | 2.546(3) |
| Na(2)-O(1)#19 | 2.432(2) | O(6)-Na(1)#25 | 2.546(3) |
| Na(2)-O(1)#6 | 2.432(2) | O(7)-O(7)#15 | 1.66(2) |
| Na(2)-O(4)#10 | 2.443(4) | O(7)-O(7)#11 | 1.66(2) |
| Na(2)-O(4)#15 | 2.443(4) | O(7)-Ca(2)#24 | 2.385(13) |
| Na(2)-O(5)#20 | 2.637(5) | O(7)-Na(1)#26 | 2.481(13) |
| Na(2)-O(5)#6 | 2.637(5) | O(7)-Na(2)#29 | 2.960(5) |
| Na(2)-O(2) | 2.700(6) | O(7)-Ca(3)#29 | 2.960(5) |
| Na(2)-C(3)#19 | 2.891(4) | O(7)-Ca(3)#24 | 2.960(5) |
| Na(2)-C(3)#6 | 2.891(4) |  |  |

Symmetry transformations used to generate equivalent atoms: #1 -x+y,-x+1,z; #2 -y+1,x-y+1,z;   
#3 -x+y,y,z; #4 x,x-y+1,z; #5 -y+1,-x+1,z; #6 y,-x+y+1,z-1/2; #7 -x+1,-y+2,z-1/2; #8 x-y+1,x+1,z-1/2;   
#9 x+1,y,z; #10 -x+y-1,y,z; #11 -x+y-1,-x+1,z; #12 -x,-y+2,z-1/2; #13 y-1,-x+y,z-1/2; #14 x,x-y+2,z;   
#15 -y+1,x-y+2,z; #16 -y+1,-x,z; #17 -x+y-1,-x,z; #18 x,y-1,z; #19 x-y,x,z-1/2; #20 x-y,-y+1,z-1/2;   
#21 x-1,y,z; #22 y,-x+y,z+1/2; #23 x-y+1,x,z+1/2; #24 -x,-y+2,z+1/2; #25 -y,x-y+1,z; #26 x,y+1,z; #27 -x+1,-y+2,z+1/2; #28 y-1,-x+y,z+1/2; #29 x-y+1,x+1,z+1/2.

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**Figure S1.** X-ray powder diffraction patterns of RbNa5Ca5(CO3)8 at 800 ℃.

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