

Table 5. Interatomic bond angles (°) for Ga/Ge sodalite.

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|-------------------|------------|-------------------|------------|
| O1#1-Ga1-O1#2 | 111.9(10) | O1#1-Ga1-O1 | 108.3(5) |
| O1#2-Ga1-O1 | 108.3(5) | O1#1-Ga1-O1#3 | 108.3(5) |
| O1#2-Ga1-O1#3 | 108.3(5) | O1-Ga1-O1#3 | 111.9(10) |
| O1#1-Ga1-Na1#3 | 37.3(9) | O1#2-Ga1-Na1#3 | 119.0(9) |
| O1-Ga1-Na1#3 | 71.4(5) | O1#3-Ga1-Na1#3 | 128.9(8) |
| O1#1-Ga1-Na1#4 | 128.9(8) | O1#2-Ga1-Na1#4 | 71.4(5) |
| O1-Ga1-Na1#4 | 37.3(9) | O1#3-Ga1-Na1#4 | 119.0(9) |
| Na1#3-Ga1-Na1#4 | 94.39(6) | O1#1-Ga1-Na1#5 | 71.4(5) |
| O1#2-Ga1-Na1#5 | 128.9(8) | O1-Ga1-Na1#5 | 119.0(9) |
| O1#3-Ga1-Na1#5 | 37.3(9) | Na1#3-Ga1-Na1#5 | 94.38(6) |
| Na1#4-Ga1-Na1#5 | 147.9(2) | O1#6-Ge1-O1#7 | 113.1(12) |
| O1#6-Ge1-O1 | 107.7(6) | O1#7-Ge1-O1 | 107.7(6) |
| O1#6-Ge1-O1#8 | 107.7(6) | O1#7-Ge1-O1#8 | 107.7(6) |
| O1-Ge1-O1#8 | 113.1(12) | O2#9-Na1-O2#10 | 81(2) |
| O2#9-Na1-O1#2 | 95.3(14) | O2#10-Na1-O1#2 | 94.1(13) |
| O2#9-Na1-O1#11 | 173.6(13) | O2#10-Na1-O1#11 | 95.3(14) |
| O1#2-Na1-O1#11 | 89.9(6) | O2#9-Na1-O1#12 | 93.9(13) |
| O2#10-Na1-O1#12 | 173.5(13) | O1#2-Na1-O1#12 | 89.8(6) |
| O1#11-Na1-O1#12 | 89.8(6) | O2#9-Na1-Na1#13 | 40.8(8) |
| O2#10-Na1-Na1#13 | 40.6(8) | O1#2-Na1-Na1#13 | 90.1(4) |
| O1#11-Na1-Na1#13 | 135.7(10) | O1#12-Na1-Na1#13 | 134.4(9) |
| O2#9-Na1-Na1#10 | 83.6(13) | O2#10-Na1-Na1#10 | 40.6(8) |
| O1#2-Na1-Na1#10 | 134.5(9) | O1#11-Na1-Na1#10 | 90.1(4) |
| O1#12-Na1-Na1#10 | 135.7(10) | Na1#13-Na1-Na1#10 | 60.0 |
| O2#9-Na1-Na1#9 | 40.6(8) | O2#10-Na1-Na1#9 | 83.5(13) |
| O1#2-Na1-Na1#9 | 135.7(10) | O1#11-Na1-Na1#9 | 134.4(9) |
| O1#12-Na1-Na1#9 | 90.1(4) | Na1#13-Na1-Na1#9 | 60.0 |
| Na1#10-Na1-Na1#9 | 60.0 | O2#9-Na1-Ga1#14 | 108.4(5) |
| O2#10-Na1-Ga1#14 | 152.4(4) | O1#2-Na1-Ga1#14 | 110.4(8) |
| O1#11-Na1-Ga1#14 | 73.1(12) | O1#12-Na1-Ga1#14 | 27.1(13) |
| Na1#13-Na1-Ga1#14 | 146.07(18) | Na1#10-Na1-Ga1#14 | 113.00(16) |
| Na1#9-Na1-Ga1#14 | 87.2(2) | O2#9-Na1-Ga1#15 | 152.6(4) |
| O2#10-Na1-Ga1#15 | 75.7(12) | O1#2-Na1-Ga1#15 | 73.1(12) |
| O1#11-Na1-Ga1#15 | 27.1(13) | O1#12-Na1-Ga1#15 | 110.5(8) |
| Na1#13-Na1-Ga1#15 | 113.04(16) | Na1#10-Na1-Ga1#15 | 87.3(2) |
| Na1#9-Na1-Ga1#15 | 146.09(18) | Ga1#14-Na1-Ga1#15 | 99.0(3) |
| Na1#10-O2-Na1#9 | 98.6(17) | Ge1-O1-Ga1 | 124.6(5) |
| Ge1-O1-Na1#4 | 118(2) | Ga1-O1-Na1#4 | 116(2) |

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, z+1/2, -y+1/2$ #2 $-x+1/2, -z+1/2, y-1/2$ #3 $x, -y+1, -z$ #4 $-y+1/2, -x+1/2, z+1/2$ #5 $-y+1/2, x+1/2, -z-1/2$ #6 $-y+1/2, x+1/2, -z+1/2$ #7 $y-1/2, -x+1/2, -z+1/2$ #8 $-x, -y+1, z$ #9 $x, -y+1, -z-1$ #10 $-x+1, y, -z-1$ #11 $-z+1/2, -y+1/2, x-1/2$ #12 $-y+1/2, -x+1/2, z-1/2$ #13 $-x+1, -y+1, z$ #14 $z, x, y-1$ #15 $-y+1, z, -x$