

**Oxynitride  $\text{K}_2\text{Ba}_{6.72}\text{Si}_{16}\text{O}_{40-1.5y}\text{N}_y:0.28 \text{Eu}^{2+}$  phosphor with high thermal stability realized by crystal field engineering**

Aijun Mao,\*<sup>a</sup> Xinwei Wang,<sup>a</sup> Yali Guo,<sup>a</sup> Xuejie Zhai,<sup>a</sup> Pai Lv<sup>a</sup>

<sup>a</sup>Department of Materials Science, School of Materials Science & Engineering,

Lanzhou Jiaotong University, Lanzhou, P.R. China

Corresponding author:maj19@mail.lzjtu.cn

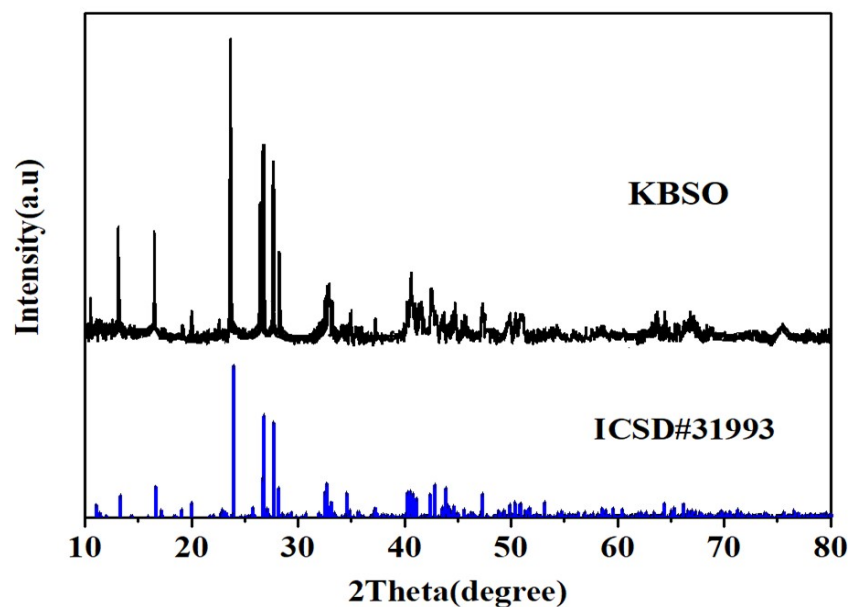


Fig.S1. XRD pattern of  $\text{K}_2\text{Ba}_7\text{Si}_{16}\text{O}_{40}$  (KBSO), together with the reference model  $\text{K}_2\text{Ba}_7\text{Si}_{16}\text{O}_{40}$  (ICSD#31993)

| Phase data         |  |      |        |            |            |             |
|--------------------|--|------|--------|------------|------------|-------------|
| <b>Space-group</b> | C 1 2/m 1 (12) - monoclinic  |      |        |            |            |             |
| <b>Cell</b>        | a=31.991(9) Å b=7.704(2) Å c=8.255(2) Å $\beta=100.60$<br>(2) <sup>o</sup> |      |        |            |            |             |
|                    | V=1999.8(9) Å <sup>3</sup> Z=2   |      |        |            |            |             |
| Atomic parameters  |  |      |        |            |            |             |
| Atom               | Wyck.  | Site | S.O.F. | x/a        | y/b        | z/c         |
| Ba1                | 4i   | m    |        | 0.1491(1)  | 0          | 0.0582(2)   |
| Ba2                | 4i   | m    |        | 0.2699(1)  | 0          | 0.8960(3)   |
| Ba3                | 4i   | m    |        | 0.3864(1)  | 0          | 0.6887(3)   |
| Ba4                | 4i   | m    | 0.333  | 0.0384(2)  | 0          | 0.2764(7)   |
| Ba5                | 2d   | 2/m  | 0.333  | 1/2        | 0          | 1/2         |
| K1                 | 4i   | m    | 0.666  | 0.0384(4)  | 0          | 0.2764(13)  |
| K2                 | 2d   | 2/m  | 0.666  | 1/2        | 0          | 1/2         |
| Si1                | 8j   | 1    |        | 0.0739(2)  | 0.2007(8)  | 0.6545(7)   |
| Si2                | 8j   | 1    |        | 0.2007(2)  | 0.2070(8)  | 0.4348(7)   |
| Si3                | 8j   | 1    |        | 0.1674(2)  | 0.2977(8)  | 0.7531(7)   |
| Si4                | 8j   | 1    |        | 0.0460(2)  | 0.2971(8)  | 0.9755(7)   |
| O1                 | 8j   | 1    |        | 0.2033(6)  | 0.2187(21) | 0.8876(18)  |
| O2                 | 8j   | 1    |        | 0.1842(6)  | 0.2761(23) | 0.2602(19)  |
| O3                 | 4i   | m    |        | 0.0572(8)  | 0          | 0.6370(27)  |
| O4                 | 4i   | m    |        | 0.1938(10) | 0          | 0.4415(36)  |
| O5                 | 4i   | m    |        | 0.3391(8)  | 0          | 0.1988(27)  |
| O6                 | 4i   | m    |        | 0.4544(8)  | 0          | -0.0369(26) |
| O7                 | 8j   | 1    |        | 0.0839(6)  | 0.2057(21) | 0.0865(19)  |
| O8                 | 8j   | 1    |        | 0.0674(5)  | 0.2892(21) | 0.4823(19)  |
| O9                 | 4g   | 2    |        | 0          | 0.2095(27) | 0           |
| O10                | 8j   | 1    |        | 0.0453(5)  | 0.2887(21) | 0.7796(18)  |
| O11                | 8j   | 1    |        | 0.1227(5)  | 0.1979(19) | 0.7592(17)  |
| O12                | 8j   | 1    |        | 0.1741(5)  | 0.296(2)   | 0.5628(17)  |
| O13                | 4f   | -1   |        | 1/4        | 1/4        | 1/2         |

Table S1. The refined phase data and atomic parameters of  $K_2Ba_7Si_{16}O_{40}$

| Phase data         |   |      |          |         |         |         |                     |
|--------------------|---|------|----------|---------|---------|---------|---------------------|
| <b>Space-group</b> | C 1 2/m 1 (12) - monoclinic   |      |          |         |         |         |                     |
| <b>Cell</b>        | a=31.72(9) Å b=7.607(23) Å c=8.333(26) Å β=101.59(6)°<br>V=1969.71(1700) Å <sup>3</sup> Z=2 |      |          |         |         |         |                     |
| Atomic parameters  |   |      |          |         |         |         |                     |
| Atom               | Wyck.   | Site | S.O.F.   | x/a     | y/b     | z/c     | U [Å <sup>2</sup> ] |
| Ba1                | 4i  | m    | 0.72(14) | 0.1491  | 0       | 0.0582  | 0.0250              |
| Ba2                | 4i  | m    | 1.02(11) | 0.2699  | 0       | 0.896   | 0.0250              |
| Ba3                | 4i  | m    |          | 0.3864  | 0       | 0.6887  | 0.0250              |
| Ba4                | 4i  | m    |          | 0.0384  | 0       | 0.2764  | 0.0250              |
| Ba5                | 2d  | 2/m  |          | 1/2     | 0       | 1/2     | 0.0250              |
| K1                 | 4i  | m    | 0.666    | 0.0384  | 0       | 0.2764  | 0.0250              |
| K2                 | 2d  | 2/m  | 0.666    | 1/2     | 0       | 1/2     | 0.0250              |
| Si1                | 8j  | 1    |          | 0.07390 | 0.20070 | 0.65450 | 0.0250              |
| Si2                | 8j  | 1    |          | 0.20070 | 0.20700 | 0.43480 | 0.0250              |
| Si3                | 8j  | 1    |          | 0.16740 | 0.29770 | 0.75310 | 0.0250              |
| Si4                | 8j  | 1    |          | 0.04600 | 0.29710 | 0.97550 | 0.0250              |
| O1                 | 8j  | 1    |          | 0.20330 | 0.21870 | 0.88760 | 0.0250              |
| O2                 | 8j  | 1    |          | 0.18420 | 0.27610 | 0.26020 | 0.0250              |
| O3                 | 4i  | m    |          | 0.0572  | 0       | 0.637   | 0.0250              |
| O4                 | 4i  | m    |          | 0.1938  | 0       | 0.4415  | 0.0250              |
| O5                 | 4i  | m    |          | 0.3391  | 0       | 0.1988  | 0.0250              |
| O6                 | 4i  | m    |          | 0.4544  | 0       | -0.0369 | 0.0250              |
| O7                 | 8j  | 1    |          | 0.08390 | 0.20570 | 0.08650 | 0.0250              |
| O8                 | 8j  | 1    |          | 0.06740 | 0.28920 | 0.48230 | 0.0250              |
| O9                 | 4g  | 2    |          | 0       | 0.2095  | 0       | 0.0250              |
| O10                | 8j  | 1    |          | 0.04530 | 0.28870 | 0.77960 | 0.0250              |
| O11                | 8j  | 1    |          | 0.12270 | 0.19790 | 0.75920 | 0.0250              |
| O12                | 8j  | 1    |          | 0.17410 | 0.29600 | 0.56280 | 0.0250              |
| O13                | 4f  | -1   |          | 1/4     | 1/4     | 1/2     | 0.0250              |
| Eu1                | 4i  | m    |          | 0.1491  | 0       | 0.0582  | 0.0250              |
| Eu2                | 4i  | m    |          | 0.2699  | 0       | 0.896   | 0.0250              |
| Eu3                | 4i  | m    |          | 0.3864  | 0       | 0.6887  | 0.0250              |
| Eu4                | 4i  | m    |          | 0.0384  | 0       | 0.2764  | 0.0250              |
| Eu5                | 2d  | 2/m  |          | 1/2     | 0       | 1/2     | 0.0250              |

Table S2. The refined phase data and atomic parameters of 0.28Eu

| Phase data  |   |
|-------------|---|
| Space-group | C 1 2/m 1 (12) - monoclinic   |
| Cell        | a=32.187(7) Å b=7.6752(18) Å c=8.2463(23) Å $\beta=100.809(22)^\circ$<br>V=2001.04(50) Å <sup>3</sup> |

| Atomic parameters |       |      |        |         |         |         |                     |
|-------------------|-------|------|--------|---------|---------|---------|---------------------|
| Atom              | Wyck. | Site | S.O.F. | x/a     | y/b     | z/c     | U [Å <sup>2</sup> ] |
| Ba1               | 4i    | m    | 0.96   | 0.1491  | 0       | 0.0582  | 0.0250              |
| Ba2               | 4i    | m    | 0.96   | 0.2699  | 0       | 0.896   | 0.0250              |
| Ba3               | 4i    | m    | 0.96   | 0.3864  | 0       | 0.6887  | 0.0250              |
| Ba4               | 4i    | m    | 0.313  | 0.0384  | 0       | 0.2764  | 0.0250              |
| Ba5               | 2d    | 2/m  | 0.313  | 1/2     | 0       | 1/2     | 0.0250              |
| K1                | 4i    | m    | 0.666  | 0.0384  | 0       | 0.2764  | 0.0250              |
| K2                | 2d    | 2/m  | 0.666  | 1/2     | 0       | 1/2     | 0.0250              |
| Si1               | 8j    | 1    | 0.85   | 0.07390 | 0.20070 | 0.65450 | 0.0250              |
| Si2               | 8j    | 1    | 0.85   | 0.20070 | 0.20700 | 0.43480 | 0.0250              |
| Si3               | 8j    | 1    | 0.85   | 0.16740 | 0.29770 | 0.75310 | 0.0250              |
| Si4               | 8j    | 1    | 0.85   | 0.04600 | 0.29710 | 0.97550 | 0.0250              |
| O1                | 8j    | 1    | 0.85   | 0.20330 | 0.21870 | 0.88760 | 0.0250              |
| O2                | 8j    | 1    | 0.85   | 0.18420 | 0.27610 | 0.26020 | 0.0250              |
| O3                | 4i    | m    | 0.85   | 0.0572  | 0       | 0.637   | 0.0250              |
| O4                | 4i    | m    | 0.85   | 0.1938  | 0       | 0.4415  | 0.0250              |
| O5                | 4i    | m    | 0.85   | 0.3391  | 0       | 0.1988  | 0.0250              |
| O6                | 4i    | m    | 0.85   | 0.4544  | 0       | -0.0369 | 0.0250              |
| O7                | 8j    | 1    | 0.85   | 0.08390 | 0.20570 | 0.08650 | 0.0250              |
| O8                | 8j    | 1    | 0.85   | 0.06740 | 0.28920 | 0.48230 | 0.0250              |
| O9                | 4g    | 2    | 0.85   | 0       | 0.2095  | 0       | 0.0250              |
| O10               | 8j    | 1    | 0.85   | 0.04530 | 0.28870 | 0.77960 | 0.0250              |
| O11               | 8j    | 1    | 0.85   | 0.12270 | 0.19790 | 0.75920 | 0.0250              |
| O12               | 8j    | 1    | 0.85   | 0.17410 | 0.29600 | 0.56280 | 0.0250              |
| O13               | 4f    | -1   | 0.85   | 1/4     | 1/4     | 1/2     | 0.0250              |
| Eu1               | 4i    | m    | 0.04   | 0.1491  | 0       | 0.0582  | 0.0250              |
| Eu2               | 4i    | m    | 0.04   | 0.2699  | 0       | 0.896   | 0.0250              |
| Eu3               | 4i    | m    | 0.04   | 0.3864  | 0       | 0.6887  | 0.0250              |
| Eu4               | 4i    | m    | 0.02   | 0.0384  | 0       | 0.2764  | 0.0250              |
| Eu5               | 2d    | 2/m  | 0.02   | 1/2     | 0       | 1/2     | 0.0250              |
| N1                | 8j    | 1    | 0.15   | 0.20330 | 0.21870 | 0.88760 | 0.0250              |
| N2                | 8j    | 1    | 0.15   | 0.18420 | 0.27610 | 0.26020 | 0.0250              |
| N3                | 4i    | m    | 0.15   | 0.0572  | 0       | 0.637   | 0.0250              |
| N4                | 4i    | m    | 0.15   | 0.1938  | 0       | 0.4415  | 0.0250              |
| N5                | 4i    | m    | 0.15   | 0.3391  | 0       | 0.1988  | 0.0250              |
| N6                | 4i    | m    | 0.15   | 0.4544  | 0       | -0.0369 | 0.0250              |
| N7                | 8j    | 1    | 0.15   | 0.08390 | 0.20570 | 0.08650 | 0.0250              |
| N8                | 8j    | 1    | 0.15   | 0.06740 | 0.28920 | 0.48230 | 0.0250              |
| N9                | 4g    | 2    | 0.15   | 0       | 0.2095  | 0       | 0.0250              |
| N10               | 8j    | 1    | 0.15   | 0.04530 | 0.28870 | 0.77960 | 0.0250              |
| N11               | 8j    | 1    | 0.15   | 0.12270 | 0.19790 | 0.75920 | 0.0250              |
| N12               | 8j    | 1    | 0.15   | 0.17410 | 0.29600 | 0.56280 | 0.0250              |
| N13               | 4f    | -1   | 0.15   | 1/4     | 1/4     | 1/2     | 0.0250              |

Table S3. The refined phase data and atomic parameters of N6



| Phase data         |  |      |        |         |         |         |                     |
|--------------------|--|------|--------|---------|---------|---------|---------------------|
| <b>Space-group</b> | C 1 2/m 1 (12) - monoclinic  |      |        |         |         |         |                     |
| <b>Cell</b>        | a=31.00(7) Å b=7.562(19) Å c=7.971(16) Å β=100.72(9)°<br>V=1835.97(1100) Å <sup>3</sup> Z=32 |      |        |         |         |         |                     |
| Atomic parameters  |  |      |        |         |         |         |                     |
| Atom               | Wyck.  | Site | S.O.F. | x/a     | y/b     | z/c     | U [Å <sup>2</sup> ] |
| Ba1                | 4i   | m    | 0.96   | 0.1491  | 0       | 0.0582  | 0.0250              |
| Ba2                | 4i   | m    | 0.96   | 0.2699  | 0       | 0.896   | 0.0250              |
| Ba3                | 4i   | m    | 0.96   | 0.3864  | 0       | 0.6887  | 0.0250              |
| Ba4                | 4i   | m    | 0.313  | 0.0384  | 0       | 0.2764  | 0.0250              |
| Ba5                | 2d   | 2/m  | 0.313  | 1/2     | 0       | 1/2     | 0.0250              |
| K1                 | 4i   | m    | 0.666  | 0.0384  | 0       | 0.2764  | 0.0250              |
| K2                 | 2d   | 2/m  | 0.666  | 1/2     | 0       | 1/2     | 0.0250              |
| Si1                | 8j   | 1    |        | 0.07390 | 0.20070 | 0.65450 | 0.0250              |
| Si2                | 8j   | 1    |        | 0.20070 | 0.20700 | 0.43480 | 0.0250              |
| Si3                | 8j   | 1    |        | 0.16740 | 0.29770 | 0.75310 | 0.0250              |
| Si4                | 8j   | 1    |        | 0.04600 | 0.29710 | 0.97550 | 0.0250              |
| O1                 | 8j   | 1    | 0.8    | 0.20330 | 0.21870 | 0.88760 | 0.0250              |
| O2                 | 8j   | 1    | 0.8    | 0.18420 | 0.27610 | 0.26020 | 0.0250              |
| O3                 | 4i   | m    | 0.8    | 0.0572  | 0       | 0.637   | 0.0250              |
| O4                 | 4i   | m    | 0.8    | 0.1938  | 0       | 0.4415  | 0.0250              |
| O5                 | 4i   | m    | 0.8    | 0.3391  | 0       | 0.1988  | 0.0250              |
| O6                 | 4i   | m    | 0.8    | 0.4544  | 0       | -0.0369 | 0.0250              |
| O7                 | 8j   | 1    | 0.8    | 0.08390 | 0.20570 | 0.08650 | 0.0250              |
| O8                 | 8j   | 1    | 0.8    | 0.06740 | 0.28920 | 0.48230 | 0.0250              |
| O9                 | 4g   | 2    | 0.8    | 0       | 0.2095  | 0       | 0.0250              |
| O10                | 8j   | 1    | 0.8    | 0.04530 | 0.28870 | 0.77960 | 0.0250              |
| O11                | 8j   | 1    | 0.8    | 0.12270 | 0.19790 | 0.75920 | 0.0250              |
| O12                | 8j   | 1    | 0.8    | 0.17410 | 0.29600 | 0.56280 | 0.0250              |
| O13                | 4f   | -1   | 0.8    | 1/4     | 1/4     | 1/2     | 0.0250              |
| Eu1                | 4i   | m    | 0.04   | 0.1491  | 0       | 0.0582  | 0.0250              |
| Eu2                | 4i   | m    | 0.04   | 0.2699  | 0       | 0.896   | 0.0250              |
| Eu3                | 4i   | m    | 0.04   | 0.3864  | 0       | 0.6887  | 0.0250              |
| Eu4                | 4i   | m    | 0.02   | 0.0384  | 0       | 0.2764  | 0.0250              |
| Eu5                | 2d   | 2/m  | 0.02   | 1/2     | 0       | 1/2     | 0.0250              |
| N1                 | 8j   | 1    | 0.2    | 0.20330 | 0.21870 | 0.88760 | 0.0250              |
| N2                 | 8j   | 1    | 0.2    | 0.18420 | 0.27610 | 0.26020 | 0.0250              |
| N3                 | 4i   | m    | 0.2    | 0.0572  | 0       | 0.637   | 0.0250              |
| N4                 | 4i   | m    | 0.2    | 0.1938  | 0       | 0.4415  | 0.0250              |
| N5                 | 4i   | m    | 0.2    | 0.3391  | 0       | 0.1988  | 0.0250              |
| N6                 | 4i   | m    | 0.2    | 0.4544  | 0       | -0.0369 | 0.0250              |
| N7                 | 8j   | 1    | 0.2    | 0.08390 | 0.20570 | 0.08650 | 0.0250              |
| N8                 | 8j   | 1    | 0.2    | 0.06740 | 0.28920 | 0.48230 | 0.0250              |
| N9                 | 4g   | 2    | 0.2    | 0       | 0.2095  | 0       | 0.0250              |
| N10                | 8j   | 1    | 0.2    | 0.04530 | 0.28870 | 0.77960 | 0.0250              |
| N11                | 8j   | 1    | 0.2    | 0.12270 | 0.19790 | 0.75920 | 0.0250              |
| N12                | 8j   | 1    | 0.2    | 0.17410 | 0.29600 | 0.56280 | 0.0250              |
| N13                | 4f   | -1   | 0.2    | 1/4     | 1/4     | 1/2     | 0.0250              |

Table S4. The refined phase data and atomic parameters of N8

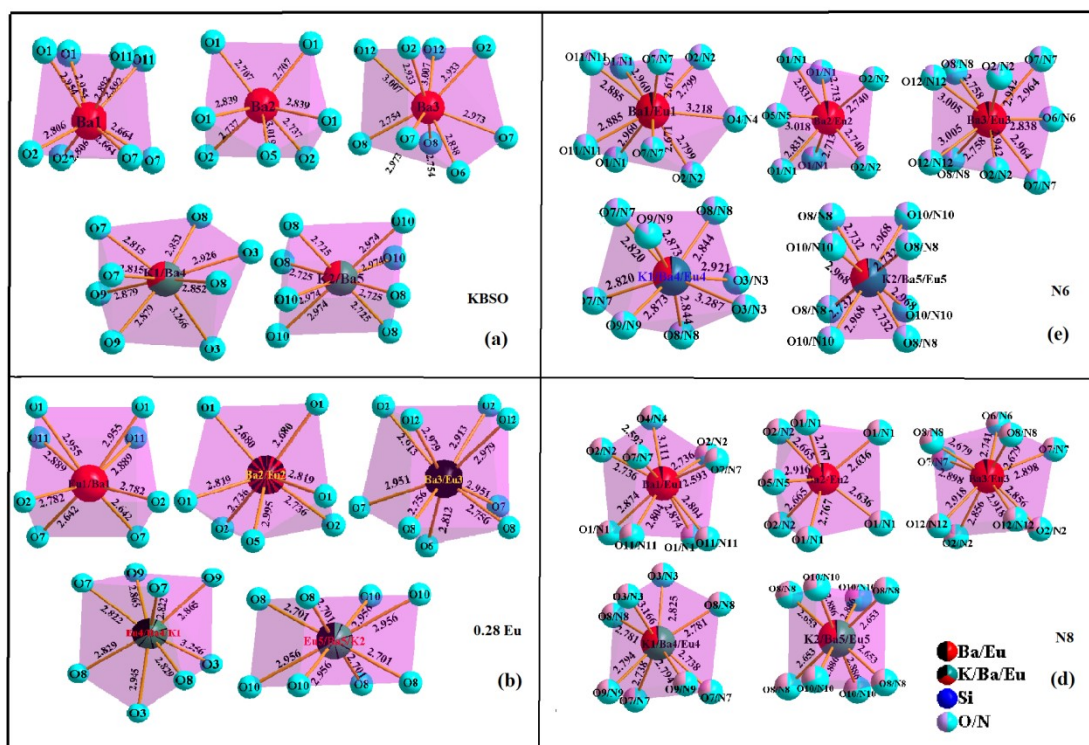


Fig.S2. the corresponding coordination environments of  $K^+/Ba^{2+}/Eu^{2+}$  in (a)  $K_2Ba_7Si_{16}O_{40}$ , (b) 0.28Eu, (c) N6, (d) N8

## Distance of Ba/Eu-O in compound lattices

### (a) Distance of Ba1/Ba2/Ba3/Ba4/Ba5-O in $K_2Ba_7Si_{16}O_{40}$

| Bond    | Length (Å) | Bond   | Length (Å) | Bond    | Length (Å) | Bond      | Length (Å) | Bond       | Length (Å) |
|---------|------------|--------|------------|---------|------------|-----------|------------|------------|------------|
| Ba1-O1  | 2.954      | Ba2-O1 | 2.707      | Ba3-O2  | 2.933      | Ba4/K1-O3 | 2.926      | Ba5/K2-O8  | 2.725      |
| Ba1-O1  | 2.954      | Ba2-O1 | 2.707      | Ba3-O2  | 2.933      | Ba4/K1-O3 | 2.926      | Ba5/K2-O8  | 2.725      |
| Ba1-O2  | 2.806      | Ba2-O1 | 2.839      | Ba3-O6  | 2.838      | Ba4/K1-O7 | 2.815      | Ba5/K2-O8  | 2.725      |
| Ba1-O2  | 2.806      | Ba2-O1 | 2.839      | Ba3-O7  | 2.973      | Ba4/K1-O7 | 2.815      | Ba5/K2-O8  | 2.725      |
| Ba1-O7  | 2.664      | Ba2-O5 | 3.019      | Ba3-O7  | 2.973      | Ba4/K1-O8 | 2.852      | Ba5/K2-O10 | 2.974      |
| Ba1-O7  | 2.664      | Ba2-O2 | 2.737      | Ba3-O8  | 2.754      | Ba4/K1-O8 | 2.852      | Ba5/K2-O10 | 2.974      |
| Ba1-O11 | 2.892      | Ba2-O2 | 2.737      | Ba3-O8  | 2.754      | Ba4/K1-O9 | 2.879      | Ba5/K2-O10 | 2.974      |
| Ba1-O11 | 2.892      |        |            | Ba3-O12 | 3.007      | Ba4/K1-O9 | 2.879      | Ba5/K2-O10 | 2.974      |
|         |            |        |            | Ba3-O12 | 3.007      |           |            |            |            |
| Average | 2.829      |        | 2.798      |         | 2.908      |           | 2.868      |            | 2.850      |

### (b) Distance of M1/M2/M3/M4/M5(M:Ba/Eu)-O in 0.28Eu

| Bond    | Length (Å) | Bond  | Length (Å) | Bond   | Length (Å) | Bond     | Length (Å) | Bond      | Length (Å) |
|---------|------------|-------|------------|--------|------------|----------|------------|-----------|------------|
| M1-O1   | 2.955      | M2-O1 | 2.680      | M3-O2  | 2.913      | M4/K1-O3 | 2.945      | M5/K2-O8  | 2.701      |
| M1-O1   | 2.955      | M2-O1 | 2.680      | M3-O2  | 2.913      | M4/K1-O3 | 2.945      | M5/K2-O8  | 2.701      |
| M1-O2   | 2.782      | M2-O1 | 2.819      | M3-O6  | 2.812      | M4/K1-O7 | 2.822      | M5/K2-O8  | 2.701      |
| M1-O2   | 2.782      | M2-O1 | 2.819      | M3-O7  | 2.951      | M4/K1-O7 | 2.822      | M5/K2-O8  | 2.701      |
| M1-O7   | 2.642      | M2-O5 | 2.995      | M3-O7  | 2.951      | M4/K1-O8 | 2.829      | M5/K2-O10 | 2.956      |
| M1-O7   | 2.642      | M2-O2 | 2.736      | M3-O8  | 2.756      | M4/K1-O8 | 2.829      | M5/K2-O10 | 2.956      |
| M1-O11  | 2.889      | M2-O2 | 2.736      | M3-O8  | 2.756      | M4/K1-O9 | 2.865      | M5/K2-O10 | 2.956      |
| M1-O11  | 2.889      |       |            | M3-O12 | 2.979      | M4/K1-O9 | 2.865      | M5/K2-O10 | 2.956      |
|         |            |       |            | M3-O12 | 2.979      |          |            |           |            |
| Average | 2.817      |       | 2.780      |        | 2.890      |          | 2.865      |           | 2.840      |



| <b>(c) Distance of M1/M2/M3/M4/M5(M:Ba/Eu)-O/N in N6</b> |           |         |           |          |           |            |           |             |           |
|--|-----------|---------|-----------|----------|-----------|------------|-----------|-------------|-----------|
| Bond   | Length(Å) | Bond    | Length(Å) | Bond     | Length(Å) | Bond       | Length(Å) | Bond        | Length(Å) |
| M1-O/N1  | 2.885     | M2-O/N1 | 2.831     | M3-O/N2  | 2.942     | M4/K1-O/N3 | 2.921     | M5/K2-O/N8  | 2.732     |
| M1-O/N1  | 2.885     | M2-O/N1 | 2.831     | M3-O/N2  | 2.942     | M4/K1-O/N3 | 2.921     | M5/K2-O/N8  | 2.732     |
| M1-O/N2  | 2.799     | M2-O/N1 | 2.713     | M3-O/N6  | 2.836     | M4/K1-O/N7 | 2.820     | M5/K2-O/N8  | 2.732     |
| M1-O/N2  | 2.799     | M2-O/N1 | 2.713     | M3-O/N7  | 2.964     | M4/K1-O/N7 | 2.820     | M5/K2-O/N8  | 2.732     |
| M1-O/N7  | 2.671     | M2-O/N5 | 3.018     | M3-O/N7  | 2.964     | M4/K1-O/N8 | 2.844     | M5/K2-O/N10 | 2.964     |
| M1-O/N7  | 2.671     | M2-O/N2 | 2.740     | M3-O/N8  | 2.758     | M4/K1-O/N8 | 2.844     | M5/K2-O/N10 | 2.963     |
| M1-O/N11   | 2.960     | M2-O/N2 | 2.740     | M3-O/N8  | 2.758     | M4/K1-O/N9 | 2.873     | M5/K2-O/N10 | 2.964     |
| M1-O/N11   | 2.960     |         |           | M3-O/N12 | 3.005     | M4/K1-O/N9 | 2.873     | M5/K2-O/N10 | 2.964     |
|  |           |         |           | M3-O/N12 | 3.005     |            |           |             |           |
| Average  | 2.828     |         | 2.798     |          | 2.907     |            | 2.864     |             | 2.848     |

| <b>(d) Distance of M1/M2/M3/M4/M5(M:Ba/Eu)-O/N in N8</b> |           |         |           |          |           |            |           |             |           |
|--|-----------|---------|-----------|----------|-----------|------------|-----------|-------------|-----------|
| Bond   | Length(Å) | Bond    | Length(Å) | Bond     | Length(Å) | Bond       | Length(Å) | Bond        | Length(Å) |
| M1-O/N1  | 2.874     | M2-O/N1 | 2.767     | M3-O/N2  | 2.856     | M4/K1-O/N3 | 2.794     | M5/K2-O/N8  | 2.653     |
| M1-O/N1  | 2.874     | M2-O/N1 | 2.767     | M3-O/N2  | 2.856     | M4/K1-O/N3 | 2.794     | M5/K2-O/N8  | 2.653     |
| M1-O/N2  | 2.736     | M2-O/N1 | 2.338     | M3-O/N6  | 2.741     | M4/K1-O/N7 | 2.738     | M5/K2-O/N8  | 2.653     |
| M1-O/N2  | 2.736     | M2-O/N1 | 2.338     | M3-O/N7  | 2.898     | M4/K1-O/N7 | 2.738     | M5/K2-O/N8  | 2.653     |
| M1-O/N7  | 2.593     | M2-O/N5 | 2.916     | M3-O/N7  | 2.898     | M4/K1-O/N8 | 2.825     | M5/K2-O/N10 | 2.886     |
| M1-O/N7  | 2.593     | M2-O/N2 | 2.665     | M3-O/N8  | 2.679     | M4/K1-O/N8 | 2.825     | M5/K2-O/N10 | 2.886     |
| M1-O/N11   | 2.804     | M2-O/N2 | 2.665     | M3-O/N8  | 2.679     | M4/K1-O/N9 | 2.781     | M5/K2-O/N10 | 2.886     |
| M1-O/N11   | 2.804     |         |           | M3-O/N12 | 2.918     | M4/K1-O/N9 | 2.781     | M5/K2-O/N10 | 2.886     |
|  |           |         |           | M3-O/N12 | 2.918     |            |           |             |           |
| Average  | 2.752     |         | 2.637     |          | 2.827     |            | 2.784     |             | 2.770     |

Table. S5 The distance of M(Ba/Eu/K)-O/N in compound (a)  $K_2Ba_7Si_{16}O_{40}$ , (b) 0.28Eu, (c) N6, (d) N8 lattice.