

Luminescence of a new class UV- blue- emitting phosphors
MSi₂O_{2- δ} N_{2+2/3 δ} :Ce³⁺ (M = Ca, Sr, Ba)

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Table 1. X-ray powder diffraction data for MSi₂O_{2- δ} N_{2+2/3 δ} (M = Ca, Sr)

(a) M = Ca ($\delta \approx 0$)

| h | k | l | d _{obs} (Å) | 2 θ _{obs} (deg.) | 2 θ _{cal} (deg.) | $\Delta 2\theta$ (deg.) | I/I _o (%) |
|---|---|----|----------------------|----------------------------------|----------------------------------|-------------------------|----------------------|
| 0 | 0 | 1 | 6.87726 | 12.862 | 12.934 | -0.072 | 33.8 |
| 1 | 1 | -1 | 5.94881 | 14.880 | 14.881 | -0.001 | 3.2 |
| 2 | 1 | -1 | 4.99010 | 17.760 | 17.710 | 0.050 | 4.5 |
| 1 | 2 | 1 | 4.75165 | 18.659 | 18.671 | -0.012 | 7.8 |
| 0 | 3 | 1 | 4.11482 | 21.579 | 21.564 | 0.015 | 16.6 |
| 1 | 4 | 0 | 3.75130 | 23.699 | 23.741 | -0.042 | 8.6 |
| 0 | 0 | 2 | 3.42184 | 26.019 | 26.045 | -0.026 | 89.0 |
| 0 | 1 | 2 | 3.33621 | 26.699 | 26.685 | 0.014 | 64.9 |
| 1 | 0 | 2 | 3.26388 | 27.302 | 27.263 | 0.039 | 8.3 |
| 1 | 1 | 2 | 3.19291 | 27.921 | 27.876 | 0.045 | 17.6 |
| 1 | 2 | -2 | 3.11022 | 28.679 | 28.656 | 0.023 | 15.8 |
| 1 | 2 | 2 | 3.00756 | 29.680 | 29.648 | 0.032 | 21.7 |
| 4 | 2 | 1 | 2.92864 | 30.499 | 30.542 | -0.043 | 21.3 |
| 3 | 1 | -2 | 2.89511 | 30.861 | 30.878 | -0.017 | 10.6 |
| 0 | 3 | 2 | 2.84840 | 31.380 | 31.370 | 0.010 | 15.9 |
| 1 | 3 | 2 | 2.75605 | 32.460 | 32.404 | 0.056 | 9.8 |
| 2 | 5 | -1 | 2.66657 | 33.581 | 33.529 | 0.052 | 91.3 |
| 1 | 4 | -2 | 2.54901 | 35.179 | 35.114 | 0.065 | 62.1 |
| 0 | 6 | 1 | 2.41504 | 37.200 | 37.238 | -0.038 | 15.3 |
| 5 | 0 | -2 | 2.36117 | 38.081 | 38.138 | -0.057 | 100.0 |
| 0 | 5 | 2 | 2.29749 | 39.179 | 39.242 | -0.063 | 24.1 |
| 0 | 1 | 3 | 2.25539 | 39.941 | 39.958 | -0.017 | 20.9 |
| 1 | 0 | 3 | 2.22339 | 40.541 | 40.551 | -0.010 | 10.9 |
| 2 | 5 | 2 | 2.15431 | 41.901 | 41.860 | 0.041 | 5.9 |
| 2 | 7 | 0 | 2.12057 | 42.600 | 42.627 | -0.027 | 5.4 |
| 0 | 7 | 1 | 2.10172 | 43.001 | 42.974 | 0.027 | 6.3 |
| 0 | 3 | 3 | 2.08236 | 43.421 | 43.378 | 0.043 | 5.0 |
| 1 | 4 | -3 | 1.96743 | 46.099 | 46.122 | -0.023 | 5.4 |
| 5 | 6 | 0 | 1.94905 | 46.559 | 46.487 | 0.072 | 8.8 |
| 5 | 6 | -1 | 1.90811 | 47.619 | 47.650 | -0.031 | 18.4 |
| 5 | 1 | -3 | 1.88136 | 48.339 | 48.309 | 0.030 | 15.6 |
| 0 | 5 | 3 | 1.83713 | 49.580 | 49.647 | -0.067 | 10.5 |
| 2 | 7 | -2 | 1.82064 | 50.060 | 50.013 | 0.047 | 6.2 |
| 3 | 8 | 0 | 1.80177 | 50.621 | 50.596 | 0.025 | 15.5 |
| 7 | 3 | -2 | 1.77306 | 51.500 | 51.491 | 0.009 | 2.5 |

Table 1. (a) $M = \text{Ca}$ ($\delta \approx 0$) (cont.)

| h | k | l | d_{obs} (Å) | $2\theta_{\text{obs}}$ (deg.) | $2\theta_{\text{cal}}$ (deg.) | $\Delta 2\theta$ (deg.) | I/I_0 (%) |
|---|----|----|----------------------|-------------------------------|-------------------------------|-------------------------|-------------|
| 5 | 0 | 3 | 1.73674 | 52.659 | 52.638 | 0.021 | 6.9 |
| 0 | 0 | 4 | 1.70788 | 53.619 | 53.581 | 0.038 | 13.7 |
| 5 | 2 | 3 | 1.69325 | 54.120 | 54.055 | 0.065 | 2.6 |
| 2 | 9 | 0 | 1.67776 | 54.661 | 54.568 | 0.093 | 10.6 |
| 0 | 9 | 1 | 1.66546 | 55.099 | 55.042 | 0.057 | 0.9 |
| 3 | 6 | -3 | 1.64999 | 55.660 | 55.665 | -0.005 | 3.6 |
| 1 | 2 | 4 | 1.64078 | 56.000 | 55.938 | 0.062 | 17.2 |
| 4 | 7 | 2 | 1.63115 | 56.360 | 56.394 | -0.034 | 6.2 |
| 2 | 9 | 1 | 1.61955 | 56.800 | 56.806 | -0.006 | 2.4 |
| 4 | 1 | -4 | 1.60101 | 57.519 | 57.499 | 0.020 | 3.7 |
| 4 | 6 | -3 | 1.59492 | 57.759 | 57.784 | -0.025 | 4.1 |
| 2 | 3 | 4 | 1.55854 | 59.240 | 59.276 | -0.036 | 29.0 |
| 4 | 6 | 3 | 1.51279 | 61.220 | 61.150 | 0.070 | 11.2 |
| 1 | 10 | -1 | 1.50480 | 61.580 | 61.606 | -0.026 | 8.4 |
| 0 | 5 | 4 | 1.49603 | 61.981 | 61.985 | -0.004 | 2.8 |
| 5 | 3 | -4 | 1.47934 | 62.759 | 62.730 | 0.029 | 5.6 |
| 2 | 10 | 1 | 1.47177 | 63.119 | 63.048 | 0.071 | 3.6 |
| 2 | 5 | 4 | 1.44473 | 64.441 | 64.434 | 0.007 | 9.4 |
| 7 | 3 | 3 | 1.43247 | 65.060 | 65.047 | 0.013 | 2.2 |
| 2 | 10 | -2 | 1.39418 | 67.079 | 67.065 | 0.014 | 3.2 |
| 2 | 6 | 4 | 1.38147 | 67.779 | 67.852 | -0.073 | 5.6 |
| 0 | 11 | 1 | 1.37647 | 68.059 | 68.001 | 0.058 | 1.6 |
| 0 | 0 | 5 | 1.36586 | 68.661 | 68.587 | 0.074 | 10.4 |
| 1 | 7 | -4 | 1.35414 | 69.340 | 69.281 | 0.059 | 3.6 |
| 0 | 2 | 5 | 1.34564 | 69.841 | 69.803 | 0.038 | 5.2 |
| 5 | 4 | 4 | 1.33999 | 70.179 | 70.174 | 0.005 | 1.8 |
| 2 | 1 | 5 | 1.32004 | 71.400 | 71.472 | -0.072 | 3.0 |
| 1 | 3 | 5 | 1.30579 | 72.301 | 72.267 | 0.034 | 2.6 |
| 0 | 11 | 2 | 1.30117 | 72.599 | 72.639 | -0.040 | 2.1 |
| 8 | 7 | 2 | 1.28592 | 73.600 | 73.667 | -0.067 | 14.5 |
| 2 | 3 | 5 | 1.28205 | 73.859 | 73.854 | 0.005 | 5.4 |
| 2 | 10 | -3 | 1.27202 | 74.540 | 74.520 | 0.020 | 6.2 |
| 1 | 8 | 4 | 1.26853 | 74.780 | 74.780 | 0.000 | 4.4 |
| 1 | 12 | 1 | 1.26106 | 75.300 | 75.339 | -0.039 | 2.7 |
| 0 | 7 | -1 | 1.23414 | 77.241 | 77.251 | -0.010 | 2.4 |
| 3 | 8 | 4 | 1.22061 | 78.259 | 78.282 | -0.023 | 1.7 |
| 0 | 11 | 3 | 1.19663 | 80.140 | 80.131 | 0.009 | 2.3 |
| 4 | 10 | 3 | 1.19218 | 80.500 | 80.496 | 0.004 | 2.9 |
| 1 | 13 | 0 | 1.18657 | 80.960 | 80.989 | -0.029 | 2.1 |
| 0 | 0 | -4 | 1.17862 | 81.621 | 81.609 | 0.012 | 3.4 |
| 2 | 13 | -1 | 1.16090 | 83.140 | 83.139 | 0.001 | 5.4 |
| 5 | 10 | 3 | 1.15454 | 83.701 | 83.633 | 0.068 | 1.8 |
| 1 | 10 | -4 | 1.14831 | 84.259 | 84.212 | 0.047 | 1.8 |
| 1 | 10 | 4 | 1.13780 | 85.220 | 85.183 | 0.037 | 1.7 |
| 1 | 8 | -5 | 1.11924 | 86.981 | 86.968 | 0.013 | 2.3 |
| 2 | 0 | 6 | 1.11130 | 87.760 | 87.760 | 0.000 | 3.4 |
| 1 | 3 | 6 | 1.10174 | 88.720 | 88.678 | 0.042 | 3.8 |

(b) M = Sr ($\delta \approx 1$)

| h | k | l | D _{obs} (Å) | 2 θ _{obs} (deg.) | 2 θ _{cal} (deg.) | $\Delta 2\theta$ (deg.) | I/I _o (%) |
|---|----|----|----------------------|----------------------------------|----------------------------------|-------------------------|----------------------|
| 0 | 2 | 0 | 7.07617 | 12.499 | 12.488 | 0.011 | 18.8 |
| 2 | 0 | 0 | 5.66933 | 15.618 | 15.596 | 0.022 | 1.2 |
| 2 | 1 | -1 | 4.42284 | 20.060 | 20.093 | -0.033 | 2.2 |
| 0 | 0 | 2 | 3.88052 | 22.899 | 22.927 | -0.028 | 2.0 |
| 0 | 4 | 0 | 3.52827 | 25.221 | 25.205 | 0.016 | 100.0 |
| 3 | 0 | -1 | 3.44003 | 25.879 | 25.890 | -0.011 | 9.4 |
| 3 | 1 | -1 | 3.34100 | 26.660 | 26.662 | -0.002 | 5.8 |
| 1 | 2 | 2 | 3.22702 | 27.620 | 27.607 | 0.013 | 8.0 |
| 2 | 1 | -2 | 3.16228 | 28.197 | 28.189 | 0.008 | 2.1 |
| 1 | 4 | -1 | 3.10376 | 28.740 | 28.771 | -0.031 | 4.8 |
| 4 | 0 | 0 | 2.83073 | 31.581 | 31.570 | 0.011 | 45.5 |
| 3 | 3 | 1 | 2.73149 | 32.760 | 32.781 | -0.021 | 2.1 |
| 2 | 3 | 2 | 2.61518 | 34.261 | 34.234 | 0.027 | 7.4 |
| 1 | 0 | -3 | 2.52959 | 35.458 | 35.398 | 0.060 | 12.5 |
| 3 | 4 | 1 | 2.43023 | 36.959 | 36.972 | -0.013 | 4.7 |
| 2 | 5 | 1 | 2.39278 | 37.559 | 37.590 | -0.031 | 12.6 |
| 0 | 6 | 0 | 2.34935 | 38.280 | 38.248 | 0.032 | 2.4 |
| 3 | 3 | 2 | 2.31446 | 38.880 | 38.862 | 0.018 | 6.9 |
| 1 | 3 | 3 | 2.20578 | 40.879 | 40.867 | 0.012 | 6.3 |
| 3 | 5 | 1 | 2.15633 | 41.860 | 41.828 | 0.032 | 2.4 |
| 5 | 2 | 1 | 2.06163 | 43.880 | 43.906 | -0.026 | 3.7 |
| 1 | 6 | 2 | 1.97151 | 45.998 | 45.976 | 0.022 | 4.1 |
| 0 | 0 | 4 | 1.93412 | 46.940 | 46.927 | 0.013 | 5.2 |
| 1 | 0 | 4 | 1.89683 | 47.920 | 47.917 | 0.003 | 1.7 |
| 2 | 7 | 1 | 1.83852 | 49.540 | 49.537 | 0.003 | 6.6 |
| 2 | 0 | 4 | 1.81460 | 50.238 | 50.288 | -0.050 | 6.0 |
| 1 | 7 | -2 | 1.76989 | 51.599 | 51.635 | -0.036 | 6.3 |
| 1 | 3 | 4 | 1.75718 | 52.000 | 51.946 | 0.054 | 3.7 |
| 6 | 3 | 0 | 1.74967 | 52.240 | 52.220 | 0.020 | 6.0 |
| 0 | 8 | 1 | 1.71678 | 53.319 | 53.265 | 0.054 | 3.8 |
| 2 | 4 | 4 | 1.61326 | 57.042 | 57.094 | -0.052 | 1.3 |
| 0 | 8 | 2 | 1.60501 | 57.362 | 57.415 | -0.053 | 2.4 |
| 1 | 5 | -4 | 1.58386 | 58.201 | 58.156 | 0.045 | 11.4 |
| 0 | 0 | 5 | 1.54854 | 59.661 | 59.721 | -0.060 | 5.6 |
| 2 | 9 | 1 | 1.47845 | 62.801 | 62.768 | 0.033 | 3.7 |
| 3 | 1 | 5 | 1.40790 | 66.340 | 66.311 | 0.029 | 4.3 |
| 1 | 5 | -5 | 1.34971 | 69.600 | 69.532 | 0.068 | 1.2 |
| 1 | 10 | 2 | 1.31242 | 71.879 | 71.807 | 0.072 | 4.3 |