**Supplementary material of**

Crystal structures and property characterization of two magnetic frustration compounds

*Kunkun Li,†, ‡ Duanduan Yuan,†, ‡ Shijie Shen,£ and Jiangang Guo\*, †*

†Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

‡University of Chinese Academy of Sciences, Beijing 100049, China

£Department of Physics & Electronic Engineering, Taizhou University, Taizhou 318000, China.

\*Corresponding Author: jgguo@iphy.ac.cn

TABLE SI. Indexed XRD data for Co0.7Al2Se3.7.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 2*θ*obs(°) | 2*θ*cal(°) | ∆2*θ*(°) | *d*obs(Å) | *d*cal(Å) | *I*obs(‰) | *hkl* |
| 6.981 | 6.973 | -0.008 | 12.651 | 12.6659 | 421 | ( 0 0 1) |
| 13.973 | 13.966 | -0.008 | 6.3326 | 6.336 | 6 | ( 0 0 2) |
| 21.019 | 21.011 | -0.008 | 4.2231 | 4.2247 | 1000 | ( 0 0 3) |
| 27.019 | 27.015 | -0.004 | 3.2974 | 3.2978 | 43 | ( 1 0 0) |
| 28.139 | 28.137 | -0.002 | 3.1685 | 3.1688 | 985 | ( 0 0 4) |
| 30.529 | 30.531 | 0.002 | 2.9257 | 2.9255 | 161 | ( 0 1 2) |
| 35.377 | 35.377 | 0 | 2.5352 | 2.5351 | 88 | ( 0 0 5) |
| 39.402 | 39.399 | -0.002 | 2.285 | 2.2851 | 73 | ( 0 1 4) |
| 42.765 | 42.766 | 0.001 | 2.1127 | 2.1127 | 6 | ( 0 0 6) |
| 45.066 | 45.066 | 0 | 2.01 | 2.01 | 45 | ( 0 1 5) |
| 47.724 | 47.721 | -0.003 | 1.9041 | 1.9042 | 60 | ( 1 1 0) |
| 50.348 | 50.346 | -0.002 | 1.8109 | 1.8109 | 8 | ( 0 0 7) |
| 51.317 | 51.313 | -0.004 | 1.7789 | 1.779 | 117 | ( 0 1 6) |
| 52.671 | 52.679 | 0.008 | 1.7363 | 1.7361 | 11 | ( 1 1 3) |
| 56.316 | 56.317 | 0.001 | 1.6323 | 1.6323 | 22 | ( 1 1 4) |
| 57.705 | 57.715 | 0.01 | 1.5963 | 1.596 | 19 | ( 0 2 2) |
| 58.17 | 58.17 | 0 | 1.5846 | 1.5846 | 86 | ( 0 0 8) |
| 63.52 | 63.542 | 0.022 | 1.4634 | 1.4629 | 8 | ( 2 0 4) |
| 65.266 | 65.271 | 0.005 | 1.4284 | 1.4283 | 6 | ( 0 1 8) |
| 66.303 | 66.304 | 0.001 | 1.4086 | 1.4085 | 6 | ( 0 0 9) |
| 67.728 | 67.723 | -0.005 | 1.3823 | 1.3824 | 5 | ( 0 2 5) |
| 72.674 | 72.67 | -0.003 | 1.3 | 1.3 | 15 | ( 0 2 6) |
| 72.974 | 72.973 | -0.001 | 1.2954 | 1.2954 | 29 | ( 1 0 9) |
| 74.843 | 74.835 | -0.008 | 1.2676 | 1.2677 | 18 | ( 0 0 10) |
| 78.055 | 78.057 | 0.002 | 1.2233 | 1.2232 | 11 | ( 1 2 2) |
| 78.442 | 78.451 | 0.009 | 1.2182 | 1.2181 | 14 | ( 1 1 8) |
| 81.229 | 81.226 | -0.003 | 1.1833 | 1.1833 | 11 | ( 1 0 10) |
| 83.184 | 83.203 | 0.019 | 1.1604 | 1.1602 | 4 | ( 1 2 4) |
| 83.874 | 83.883 | 0.009 | 1.1526 | 1.1525 | 23 | ( 0 0 11) |
| 88.951 | 88.949 | -0.003 | 1.0994 | 1.0995 | 6 | ( 3 0 0) |
| 90.14 | 90.143 | 0.003 | 1.088 | 1.088 | 9 | ( 0 1 11) |
| 91.675 | 91.68 | 0.004 | 1.0738 | 1.0737 | 11 | ( 1 2 6) |
| 91.977 | 91.969 | -0.007 | 1.071 | 1.0711 | 8 | ( 0 2 9) |
| 93.629 | 93.626 | -0.003 | 1.0564 | 1.0564 | 8 | ( 0 0 12) |
| 93.808 | 93.76 | -0.048 | 1.0549 | 1.0553 | 5 | ( 1 1 10) |
| 99.913 | 99.922 | 0.009 | 1.0062 | 1.0061 | 7 | ( 1 0 12) |
| 102.723 | 102.745 | 0.022 | 0.9861 | 0.986 | 11 | ( 1 1 11) |
| 107.954 | 107.988 | 0.034 | 0.9524 | 0.9522 | 5 | ( 2 2 0) |
| 110.91 | 110.908 | -0.003 | 0.9352 | 0.9352 | 10 | ( 0 1 13) |
| 111.263 | 111.194 | -0.069 | 0.9332 | 0.9336 | 7 | ( 2 1 9) |
| 131.397 | 131.393 | -0.003 | 0.8452 | 0.8452 | 9 | ( 0 0 15) |
| 133.133 | 133.128 | -0.005 | 0.8395 | 0.8395 | 7 | ( 3 1 6) |

TABLE SII. Indexed XRD data for NiAl2Se3.7.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 2*θ*obs(°) | 2*θ*cal(°) | ∆2*θ*(°) | *d*obs(Å) | *d*cal(Å) | *I*obs(‰) | *hkl* |
| 6.929 | 6.904 | -0.025 | 12.7473 | 12.7933 | 128 | ( 0 0 1) |
| 13.87 | 13.911 | 0.04 | 6.3793 | 6.3609 | 7 | ( 0 0 2) |
| 20.983 | 20.971 | -0.012 | 4.2303 | 4.2326 | 205 | ( 0 0 3) |
| 27.084 | 27.079 | -0.005 | 3.2896 | 3.2902 | 273 | ( 1 0 0) |
| 28.119 | 28.113 | -0.006 | 3.1708 | 3.1715 | 224 | ( 0 0 4) |
| 30.594 | 30.594 | -0.001 | 2.9197 | 2.9197 | 1000 | ( 1 0 2) |
| 35.373 | 35.369 | -0.004 | 2.5354 | 2.5357 | 21 | ( 0 0 5) |
| 39.467 | 39.466 | -0.001 | 2.2813 | 2.2814 | 255 | ( 1 0 4) |
| 45.147 | 45.139 | -0.007 | 2.0066 | 2.0069 | 100 | ( 0 1 5) |
| 47.907 | 47.91 | 0.003 | 1.8973 | 1.8972 | 360 | ( 1 1 0) |
| 48.461 | 48.479 | 0.018 | 1.8769 | 1.8762 | 10 | ( 1 1 1) |
| 51.399 | 51.396 | -0.002 | 1.7763 | 1.7764 | 236 | ( 0 1 6) |
| 52.87 | 52.868 | -0.002 | 1.7303 | 1.7303 | 52 | ( 1 1 3) |
| 55.929 | 55.932 | 0.003 | 1.6427 | 1.6426 | 28 | ( 2 0 0) |
| 56.512 | 56.509 | -0.003 | 1.6271 | 1.6272 | 103 | ( 1 1 4) |
| 57.964 | 57.957 | -0.007 | 1.5897 | 1.5899 | 121 | ( 0 2 2) |
| 58.132 | 58.153 | 0.021 | 1.5855 | 1.585 | 82 | ( 1 0 7) |
| 60.974 | 60.978 | 0.005 | 1.5183 | 1.5182 | 14 | ( 1 1 5) |
| 63.784 | 63.79 | 0.007 | 1.458 | 1.4578 | 42 | ( 2 0 4) |
| 65.373 | 65.385 | 0.011 | 1.4263 | 1.4261 | 8 | ( 0 1 8) |
| 67.976 | 67.977 | 0.001 | 1.3779 | 1.3779 | 20 | ( 0 2 5) |
| 72.939 | 72.935 | -0.005 | 1.2959 | 1.296 | 58 | ( 0 2 6) |
| 74.927 | 74.933 | 0.006 | 1.2664 | 1.2663 | 7 | ( 0 0 10) |
| 76.732 | 76.722 | -0.009 | 1.241 | 1.2412 | 17 | ( 2 1 0) |
| 78.47 | 78.462 | -0.008 | 1.2178 | 1.2179 | 76 | ( 2 1 2) |
| 78.688 | 78.688 | 0 | 1.215 | 1.215 | 76 | ( 1 1 8) |
| 81.395 | 81.388 | -0.007 | 1.1813 | 1.1814 | 10 | ( 0 1 10) |
| 83.632 | 83.622 | -0.01 | 1.1553 | 1.1554 | 32 | ( 1 2 4) |
| 83.916 | 84.013 | 0.097 | 1.1521 | 1.151 | 17 | ( 0 0 11) |
| 85.96 | 85.978 | 0.018 | 1.1299 | 1.1297 | 4 | ( 1 1 9) |
| 87.429 | 87.457 | 0.028 | 1.1146 | 1.1143 | 14 | ( 1 2 5) |
| 89.469 | 89.471 | 0.002 | 1.0944 | 1.0944 | 30 | ( 3 0 0) |
| 90.335 | 90.34 | 0.004 | 1.0862 | 1.0861 | 9 | ( 1 0 11) |
| 92.126 | 92.131 | 0.005 | 1.0697 | 1.0696 | 50 | ( 1 2 6) |
| 93.244 | 93.296 | 0.051 | 1.0598 | 1.0593 | 7 | ( 0 3 3) |
| 94.065 | 94.055 | -0.01 | 1.0527 | 1.0528 | 8 | ( 1 1 10) |
| 96.299 | 96.28 | -0.018 | 1.0341 | 1.0342 | 16 | ( 3 0 4) |
| 97.672 | 97.676 | 0.004 | 1.0232 | 1.0232 | 7 | ( 2 1 7) |
| 100.136 | 100.144 | 0.008 | 1.0045 | 1.0045 | 8 | ( 3 0 5) |
| 103.088 | 103.087 | -0.001 | 0.9836 | 0.9837 | 17 | ( 1 1 11) |
| 108.768 | 108.756 | -0.012 | 0.9475 | 0.9476 | 15 | ( 2 2 0) |
| 111.237 | 111.215 | -0.022 | 0.9333 | 0.9335 | 8 | ( 0 1 13) |
| 111.759 | 111.77 | 0.011 | 0.9304 | 0.9304 | 16 | ( 1 2 9) |
| 116.104 | 116.118 | 0.014 | 0.9078 | 0.9077 | 13 | ( 2 2 4) |
| 117.492 | 117.485 | -0.008 | 0.901 | 0.9011 | 23 | ( 1 3 2) |
| 120.518 | 120.486 | -0.031 | 0.8871 | 0.8873 | 5 | ( 2 0 12) |
| 123.39 | 123.404 | 0.014 | 0.8749 | 0.8748 | 13 | ( 1 3 4) |
| 128.071 | 128.121 | 0.05 | 0.8568 | 0.8566 | 8 | ( 1 3 5) |