

## Supporting Information

### Syntheses, structures, and magnetic properties of three new chain compounds based on the pentagonal bipyramidal Co(II) building block

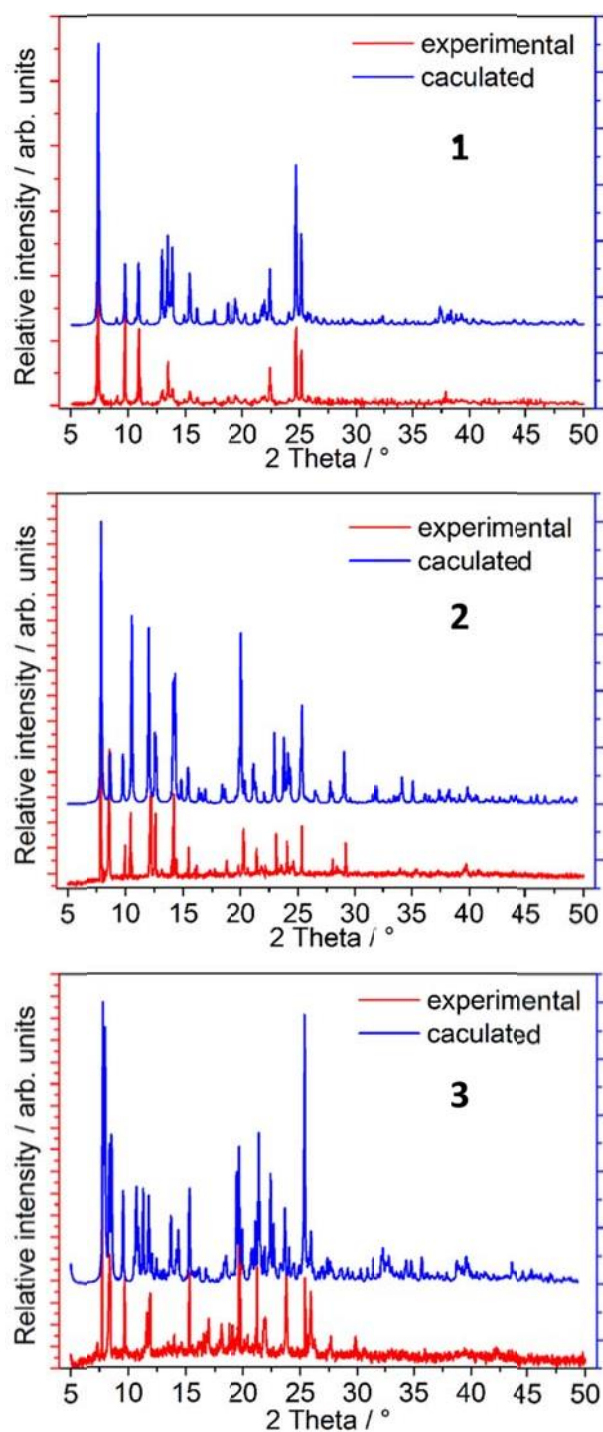
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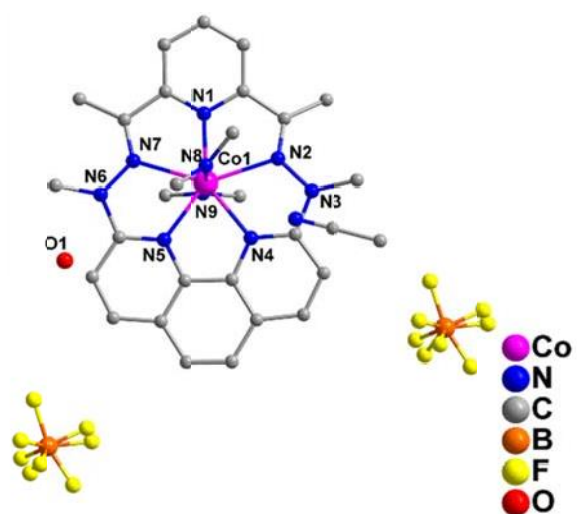
#### Table of Contents

|                                                                                                        |    |
|--------------------------------------------------------------------------------------------------------|----|
| <b>Figure S1.</b> The PXRD of <b>1-3</b> .....                                                         | 2  |
| <b>Figure S2.</b> The asymmetric units of <b>1-3</b> .....                                             | 3  |
| <b>Figure S3.</b> The packing crystal structures of <b>1-3</b> .....                                   | 4  |
| <b>Figure S4.</b> Temperature dependence of ac magnetic susceptibility for <b>1</b> and <b>2</b> ..... | 5  |
| <b>Figure S5.</b> The magnetization curves of <b>1</b> and <b>2</b> .....                              | 6  |
| <b>Figure S6.</b> Frequency dependence of ac magnetic susceptibility for <b>3</b> .....                | 7  |
| <b>Figure S7.</b> Temperature-dependent ac signals for <b>3</b> .....                                  | 8  |
| <b>Table S1.</b> Selected bond lengths (Å) and angles (°) for <b>1-3</b> .....                         | 9  |
| <b>Table S2.</b> Relaxation fitting parameters of the Cole-Cole plots of <b>3</b> .....                | 10 |

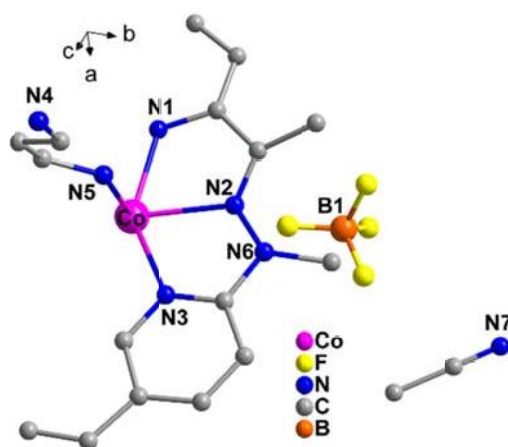


**Figure S1** | The PXRD of 1-3.

1



2



3

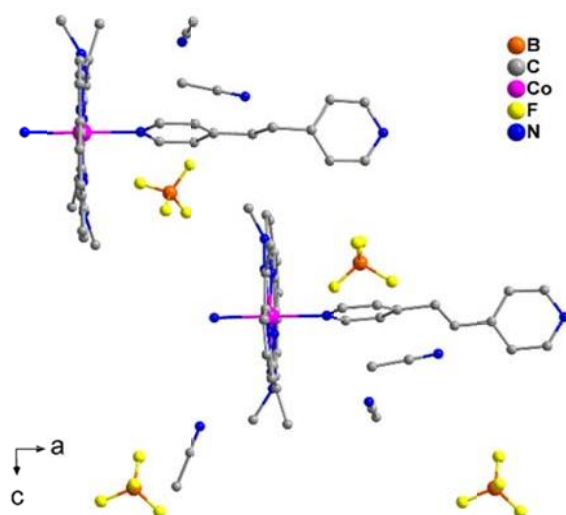
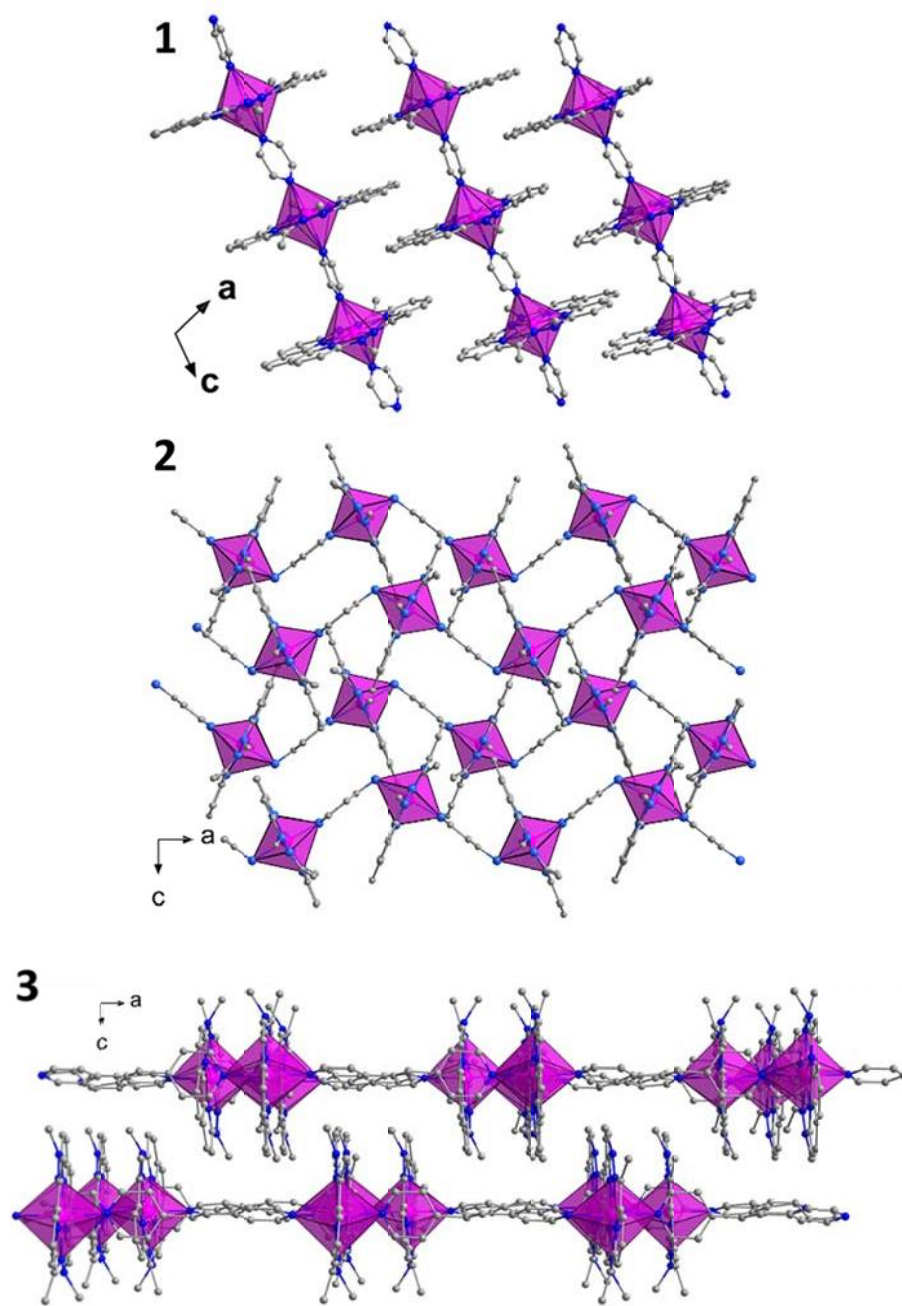
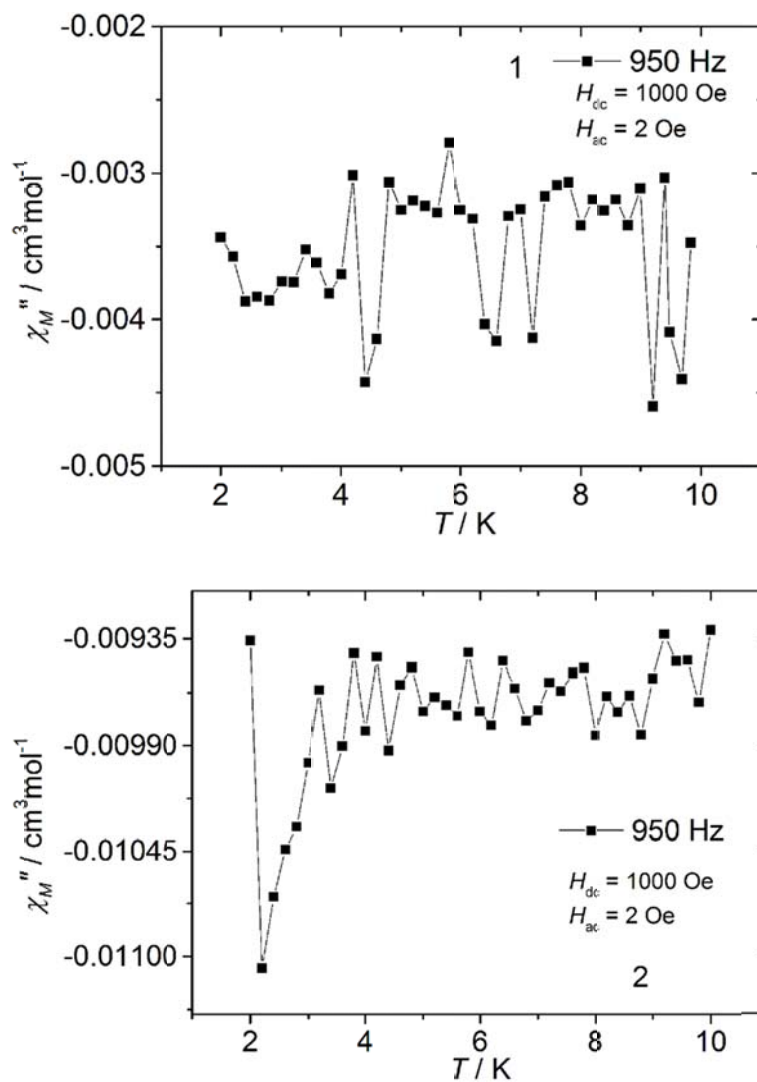


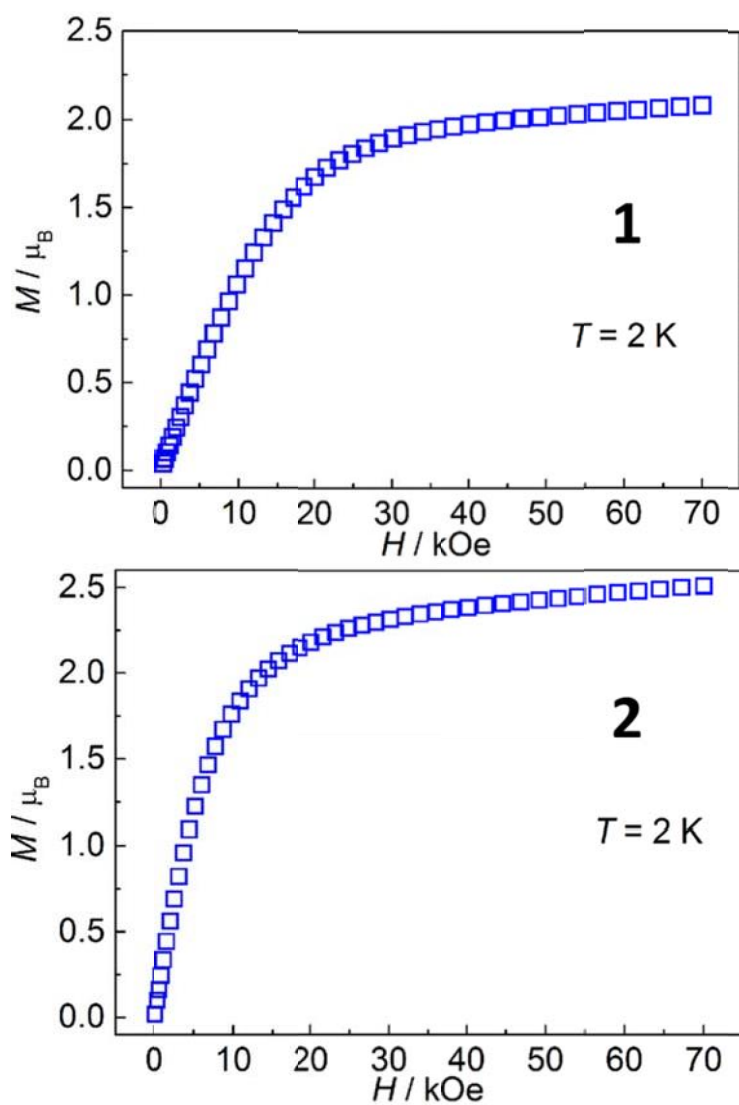
Figure S2 | The asymmetric units of 1-3.



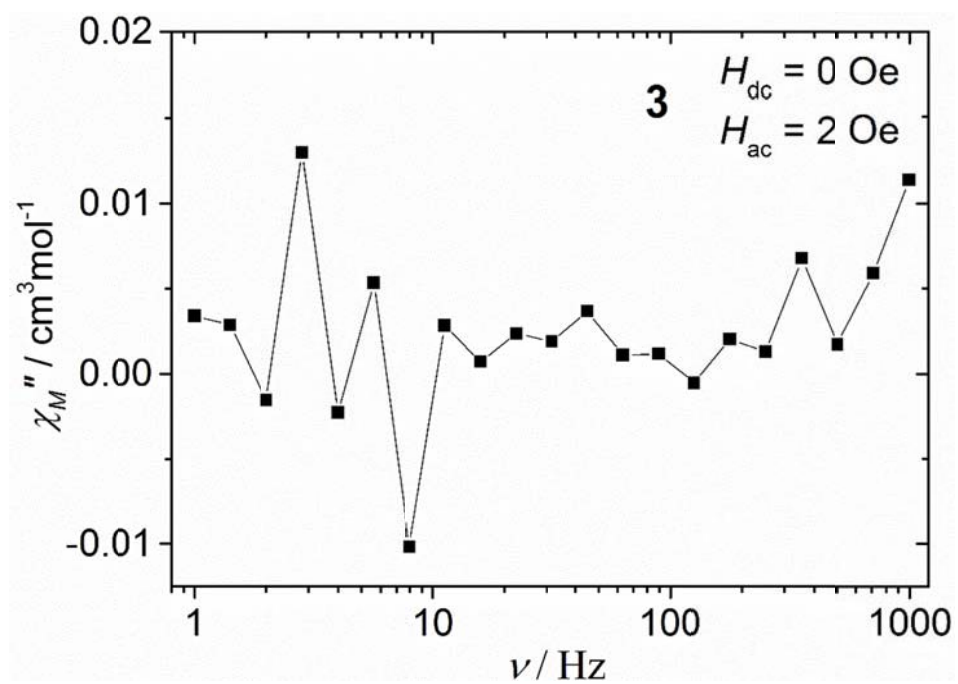
**Figure S3** | The packing crystal structures of **1-3**.



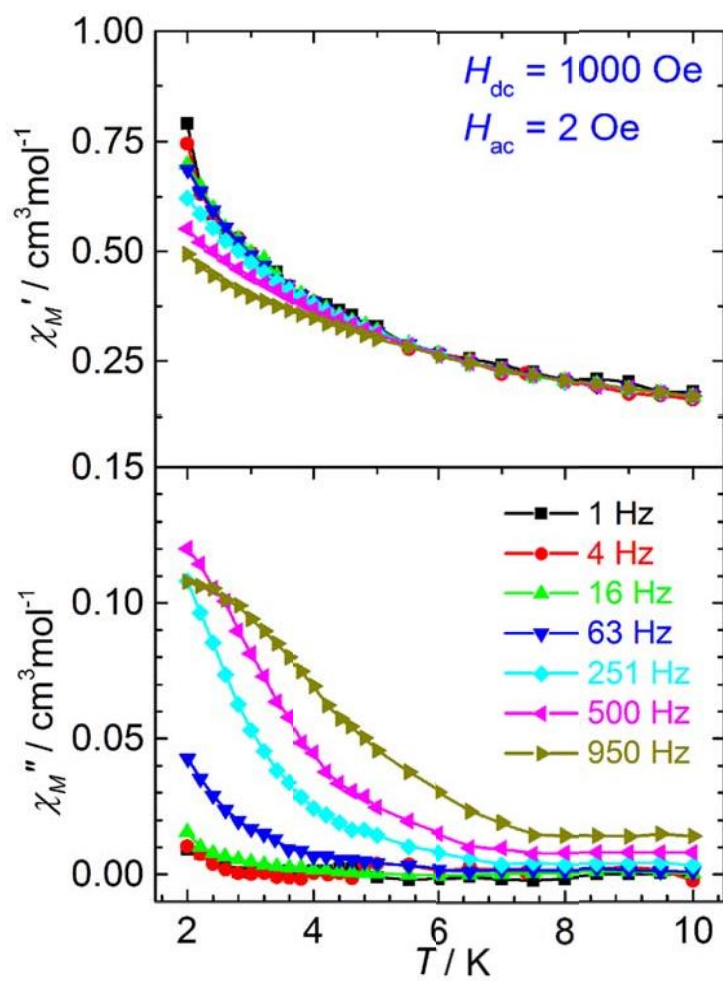
**Figure S4** | Temperature dependence of the out-of-phase ( $\chi''$ ) part of the ac magnetic susceptibility for **1** and **2** in 1 kOe dc field, oscillating at 950 Hz.



**Figure S5** | The magnetization curves of **1** and **2** measured at 2.0 K.



**Figure S6** | Frequency dependence of out-of-phase ( $\chi''$ ) part of the ac magnetic susceptibility for **3** in 1 kOe dc field at 2 K.



**Figure S7** | Temperature-dependent of in-of-phase ( $\chi'$ ) and out-of-phase ( $\chi''$ ) part ac signals under an applied field of 1 kOe for **3**.

**Table S1.** Selected bond lengths (Å) and angles (°) for **1-3**.

| <b>1</b>                                                                    |            |             |           |           |           |
|-----------------------------------------------------------------------------|------------|-------------|-----------|-----------|-----------|
| Co1-N1                                                                      | 2.098(5)   | Co1-N5      | 2.112(5)  | Co1-N8    | 2.211(4)  |
| Co1-N2                                                                      | 2.255(5)   | Co1-N7      | 2.260(5)  | Co1-N9    | 2.274(4)  |
| Co1-N4                                                                      | 2.115(5)   |             |           |           |           |
| N8-Co1-N9                                                                   | 174.71(16) | N4-Co1-N8   | 96.73(17) | N4-Co1-N9 | 88.40(17) |
| N2-Co1-N7                                                                   | 88.32(16)  | N5-Co1-N8   | 94.72(17) | N5-Co1-N9 | 87.77(17) |
| <b>2</b>                                                                    |            |             |           |           |           |
| Co1-N1                                                                      | 2.091(3)   | Co1-N4      | 2.343(3)  | Co1-N2#1  | 2.263(2)  |
| Co1-N2                                                                      | 2.263(2)   | Co1-N5      | 2.208(3)  | Co1-N3#1  | 2.119(2)  |
| Co1-N3                                                                      | 2.115(5)   |             |           |           |           |
| N5-Co1-N4                                                                   | 178.60(12) | N5-Co1-N2#1 | 92.90(7)  | N5-Co1-N2 | 92.90(7)  |
| N3#1-Co1-N<br>2                                                             | 145.06(10) | N1-Co1-N4   | 87.38(12) | N3-Co1-N4 | 93.19(9)  |
| #1 x,-y+1/2,z; #2 x+1/2,y,-z+3/2; #3 x+1/2,-y+1/2,-z+3/2; #4 x-1/2,y,-z+3/2 |            |             |           |           |           |
| <b>3</b>                                                                    |            |             |           |           |           |
| Co1-N1                                                                      | 2.090(6)   | Co1-N4      | 2.117(0)  | Co1-N8    | 2.235(5)  |
| Co1-N2                                                                      | 2.236(9)   | Co1-N5      | 2.118(1)  | Co1-N9    | 2.243(2)  |
| Co1-N3                                                                      | 2.260(0)   | 2.289(4)    |           |           |           |
| N8-Co1-N9                                                                   | 179.67(81) | N1-Co1-N9   | 90.49(61) | N1-Co1-N8 | 89.76(01) |
| N4-Co1-N51                                                                  | 75.16(21)  | N2-Co1-N4   | 69.61(81) | N5-Co1-N9 | 89.13(71) |

**Table S2.** Relaxation fitting parameters from the least-square fitting of the Cole-Cole plots of **3** according to the generalized Debye model.

| T / K | $\chi_S / \text{cm}^3\text{mol}^{-1}\text{K}$ | $\chi_T / \text{cm}^3\text{mol}^{-1}\text{K}$ | $\tau / \text{s}$ | $\alpha$ |
|-------|-----------------------------------------------|-----------------------------------------------|-------------------|----------|
| 1.8   | 0.49941                                       | 0.77122                                       | 0.00090           | 0.15390  |
| 2.0   | 0.47053                                       | 0.73140                                       | 0.00082           | 0.15067  |
| 2.2   | 0.44748                                       | 0.65042                                       | 0.00074           | 0.14496  |
| 2.5   | 0.42395                                       | 0.58264                                       | 0.00062           | 0.12748  |
| 2.8   | 0.39346                                       | 0.52406                                       | 0.00055           | 0.15363  |
| 3.1   | 0.39030                                       | 0.49462                                       | 0.00042           | 0.14528  |
| 3.4   | 0.35782                                       | 0.46622                                       | 0.00035           | 0.15351  |
| 3.7   | 0.34598                                       | 0.42436                                       | 0.00030           | 0.14842  |
| 4.0   | 0.32097                                       | 0.36229                                       | 0.00021           | 0.14868  |
| 4.3   | 0.31140                                       | 0.34628                                       | 0.00012           | 0.14827  |