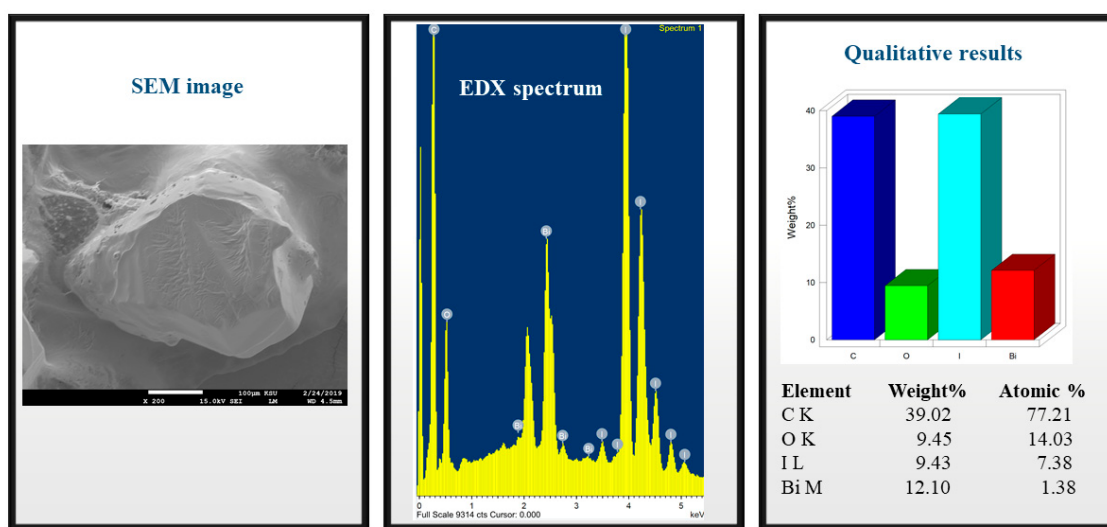


Article

# Structural, Hirshfeld Surface Analysis, Morphological Approach, and Spectroscopic Study of New Hybrid Iodobismuthate Containing Tetranuclear 0D Cluster $\text{Bi}_4\text{I}_{16}\cdot 4(\text{C}_6\text{H}_9\text{N}_2)\cdot 2(\text{H}_2\text{O})$

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**Figure S1.** SEM image, EDS spectrum and qualitative results of  $\text{Bi}_4\text{I}_{16}\cdot 4(\text{C}_6\text{H}_9\text{N}_2)\cdot 2(\text{H}_2\text{O})$  single crystal.

**Table S1.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ).

| Atoms | x           | y            | z           | <sup>a</sup> U <sub>eq</sub> |
|-------|-------------|--------------|-------------|------------------------------|
| Bi1   | 0.31035 (3) | 0.508861 (1) | 0.32032 (3) | 0.02429 (8)                  |
| Bi2   | 0.38245 (3) | 0.617864 (1) | 0.65808 (3) | 0.02630 (9)                  |
| I1    | 0.10342 (6) | 0.44051 (2)  | 0.19049 (6) | 0.04490 (2)                  |
| I2    | 0.47144 (6) | 0.48074 (2)  | 0.17239 (5) | 0.03532 (1)                  |
| I3    | 0.20571 (7) | 0.59458 (3)  | 0.16041 (7) | 0.05413 (2)                  |
| I4    | 0.54626 (5) | 0.582620 (2) | 0.48411 (5) | 0.02805 (1)                  |
| I5    | 0.16891 (5) | 0.53897 (2)  | 0.49685 (5) | 0.03740 (1)                  |
| I6    | 0.25823 (7) | 0.70246 (3)  | 0.50496 (8) | 0.0671 (2)                   |
| I7    | 0.59206 (6) | 0.68481 (2)  | 0.80004 (6) | 0.04436 (2)                  |
| I8    | 0.24247 (7) | 0.62457 (3)  | 0.82042 (7) | 0.0630 (2)                   |
| N1    | 0.6967 (7)  | 0.5916 (3)   | 0.1429 (7)  | 0.0373 (2)                   |
| N2    | 0.8550 (9)  | 0.5545 (4)   | 0.1219 (1)  | 0.070 (3)                    |

|            |            |            |             |            |
|------------|------------|------------|-------------|------------|
| <b>N3</b>  | 0.3033 (7) | 0.7764 (3) | 0.0299 (7)  | 0.0417 (2) |
| <b>N4</b>  | 0.4019 (9) | 0.8129 (4) | −0.0699 (9) | 0.067 (3)  |
| <b>C1</b>  | 0.5557 (1) | 0.7019 (7) | 0.2077 (1)  | 0.126 (8)  |
| <b>C2</b>  | 0.5993 (1) | 0.6752 (5) | 0.1508 (1)  | 0.082 (4)  |
| <b>C3</b>  | 0.5795 (1) | 0.6217 (4) | 0.1155 (1)  | 0.058 (3)  |
| <b>C4</b>  | 0.7521 (1) | 0.5638 (4) | 0.2438 (1)  | 0.054 (3)  |
| <b>C5</b>  | 0.8501 (1) | 0.5400 (4) | 0.2312 (1)  | 0.056 (3)  |
| <b>C6</b>  | 0.7619 (1) | 0.5857 (4) | 0.0696 (9)  | 0.053 (3)  |
| <b>C7</b>  | 0.0178 (1) | 0.7082 (5) | −0.0522 (1) | 0.063 (3)  |
| <b>C8</b>  | 0.0896 (9) | 0.7437 (4) | 0.0047 (1)  | 0.050 (3)  |
| <b>C9</b>  | 0.2283 (1) | 0.7362 (4) | 0.0650 (1)  | 0.053 (3)  |
| <b>C10</b> | 0.3382 (1) | 0.8220 (4) | 0.0789 (1)  | 0.063 (3)  |
| <b>C11</b> | 0.4006 (1) | 0.8460 (5) | 0.0185 (1)  | 0.072 (4)  |
| <b>C12</b> | 0.3434 (1) | 0.7711 (4) | −0.0614 (1) | 0.053 (3)  |
| <b>O1W</b> | 0.4649 (9) | 0.8239 (4) | 0.7240 (9)  | 0.093 (3)  |

$$^a U_{eq} = 1/3 \sum_i \sum_j U_{ij} a_i a_j a_i^* a_j^*$$