

Table S1. Selected crystallographic data and structure refinement for **1-4**

| Compound | 1 | 2 | 3 | 4 |
|---|---|--|--|---|
| Empirical formula | C ₆ H ₁₂ ZnN ₁₀ O ₈ | C ₁₆ H ₁₂ ZnN ₁₀ O ₄ | C ₆ H ₁₄ ZnN ₉ O ₉ | C ₃₆ H ₇₀ Zn ₃ N ₂₄ O ₃₂ |
| Formula mass | 417.65 | 473.75 | 421.65 | 1547.27 |
| Crystal system | triclinic | monoclinic | triclinic | triclinic |
| Space group | <i>P</i> $\bar{1}$ | <i>C</i> 2/ <i>c</i> | <i>P</i> $\bar{1}$ | <i>P</i> $\bar{1}$ |
| <i>a</i> (Å) | 6.1124(12) | 22.524(4) | 9.1851(18) | 8.5225(17) |
| <i>b</i> (Å) | 6.6178(13) | 8.6370(17) | 9.2931(19) | 13.641(3) |
| <i>c</i> (Å) | 9.6089(19) | 9.758(2) | 11.060(2) | 14.685(3) |
| α (°) | 78.70(3) | 90.00 | 107.50(3) | 65.49(3) |
| β (°) | 82.88(3) | 113.25(3) | 95.43(3) | 77.19(3) |
| γ (°) | 75.59(3) | 90.00 | 118.39(3) | 79.62(3) |
| <i>V</i> (Å ³) | 368.00(13) | 1744.2(6) | 759.7(3) | 1507.2(5) |
| <i>Z</i> | 1 | 4 | 2 | 1 |
| <i>T</i> /K | 291(2) | 291(2) | 291(2) | 293(2) |
| <i>D</i> _{calcd} (g.cm ⁻³) | 1.885 | 1.804 | 1.843 | 1.705 |
| μ (mm ⁻¹) | 1.737 | 1.463 | 1.687 | 1.297 |
| Reflections collected | 3869 | 8640 | 7958 | 11753 |
| Unique Reflections(<i>R</i> _{int}) | 1677 (0.0283) | 2004 (0.0860) | 3464 (0.1072) | 4767 (0.0719) |

| | | | | |
|--|----------------|----------------|----------------|----------------|
| No. Observations ($I > 2.00$) | 1557 | 1502 | 1920 | 3403 |
| $\sigma(I)$ | | | | |
| No. Variables | 115 | 141 | 211 | 421 |
| $R_1^{[a]}$, $wR_2^{[b]}$ ($I > 2\sigma(I)$) | 0.0430, 0.1506 | 0.0610, 0.1059 | 0.0758, 0.1642 | 0.0726, 0.1723 |
| R_1 , wR_2 (all data) | 0.0470, 0.1530 | 0.0910, 0.1157 | 0.1585, 0.2011 | 0.1044, 0.1904 |
| GOF ^c | 1.244 | 1.063 | 0.996 | 0.908 |
| Δ/ρ_{\max} ($e/\text{\AA}^3$) | 0.923 | 0.406 | 0.611 | 1.313 |
| Δ/ρ_{\min} ($e/\text{\AA}^3$) | -0.827 | -0.482 | -0.698 | -0.957 |

[a] $R = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$. [b] $R_w = \{ \sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2 \}^{1/2}$. [c] $GOF = \{ w((F_o^2 - F_c^2)^2) / (n-p) \}^{1/2}$, where n = number of reflections and p = total numbers of parameters refined.