

## Supplementary material

### On the importance of $\text{RH}_3\text{C}\cdots\text{N}$ tetrel bonding interactions in the solid state of a dinuclear zinc complex with a tetradentate Schiff base ligand

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**Table S1:** Crystal data and refinement details of the complex

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|--|--|
| Formula                                | $\text{C}_{18}\text{H}_{31}\text{N}_{11}\text{O}_5\text{S}_2\text{Zn}_2$ |
| Formula Weight                         | 676.44   |
| Temperature (K)                        | 273  |
| Crystal System                         | Triclinic  |
| Space group                            | <i>P</i> -1  |
| a (Å)                                  | 9.2129(9)  |
| b (Å)                                  | 9.9156(10)   |
| c (Å)                                  | 17.7795(18)  |
| $\alpha$ (°)                           | 80.589(3)  |
| $\beta$ (°)                            | 77.092(3)  |
| $\gamma$ (°)                           | 64.355(3)  |
| V(Å <sup>3</sup> )                     | 1423.1(2)  |
| Z                                      | 2  |
| $d_{\text{cal}}$ (g cm <sup>-3</sup> ) | 1.579  |
| $\mu$ (mm <sup>-1</sup> )              | 1.882  |
| F(000)                                 | 696  |
| Total reflection                       | 39040  |

|   |                |
|---|----------------|
| Unique Reflections                                  | 5066           |
| Observe data[ $I > 2\sigma(I)$ ]                    | 4579           |
| R(int)  | 0.0409         |
| R1, wR2 (all data)                                  | 0.0322, 0.0751 |
| R1, wR2 [ $I > 2\sigma(I)$ ]                        | 0.0280, 0.0718 |
| Residual Electron Density<br>( $e\text{\AA}^{-3}$ ) | 0.0373, -0.508 |

**Table S2:** Selected bond lengths ( $\text{\AA}$ ) of the complex

|            |            |
|------------|------------|
| Zn(1)-O(2) | 2.1460(18) |
| Zn(1)-O(3) | 2.1173(17) |
| Zn(1)-O(4) | 2.1160(18) |
| Zn(1)-N(1) | 2.266(2)   |
| Zn(1)-N(2) | 2.071(2)   |
| Zn(1)-N(3) | 2.146(2)   |
| Zn(2)-O(4) | 1.979(2)   |
| Zn(2)-O(5) | 2.361(2)   |
| Zn(2)-N(3) | 2.153(2)   |
| Zn(2)-N(6) | 1.955(5)   |
| Zn(2)-N(9) | 1.966(3)   |

**Table S3:** Selected bond angles ( $^\circ$ ) of the complex.

|                 |           |                 |            |
|-----------------|-----------|-----------------|------------|
| O(2)-Zn(1)-O(3) | 172.38(7) | N(1)-Zn(1)-N(3) | 115.90(8)  |
| O(2)-Zn(1)-O(4) | 95.31(7)  | N(2)-Zn(1)-N(3) | 161.39(8)  |
| O(2)-Zn(1)-N(1) | 88.84(7)  | O(4)-Zn(2)-O(5) | 72.21(8)   |
| O(2)-Zn(1)-N(2) | 89.23(8)  | O(4)-Zn(2)-N(3) | 79.81(8)   |
| O(2)-Zn(1)-N(3) | 88.45(8)  | O(4)-Zn(2)-N(6) | 123.01(16) |
| O(3)-Zn(1)-O(4) | 90.52(7)  | O(4)-Zn(2)-N(9) | 122.34(10) |
| O(3)-Zn(1)-N(1) | 86.57(7)  | O(5)-Zn(2)-N(3) | 151.74(8)  |
| O(3)-Zn(1)-N(2) | 96.20(8)  | O(5)-Zn(2)-N(6) | 92.34(16)  |
| O(3)-Zn(1)-N(3) | 88.09(8)  | O(5)-Zn(2)-N(9) | 86.45(10)  |

|                 |           |                 |            |
|-----------------|-----------|-----------------|------------|
| O(4)-Zn(1)-N(1) | 166.59(7) | N(3)-Zn(2)-N(6) | 106.41(15) |
| O(4)-Zn(1)-N(2) | 84.81(8)  | N(3)-Zn(2)-N(9) | 105.77(10) |
| O(4)-Zn(1)-N(3) | 77.04(8)  | N(6)-Zn(2)-N(9) | 110.42(17) |
| N(1)-Zn(1)-N(2) | 82.50(8)  |                 |            |