Synthesis and structure of the hexameric, dodecanuclear metallamacrocycle [(5,3-methylphenylpyrazole)$_2$Zn$_2$(OCH$_2$CH$_2$S)]$_6$

Supplementary Information

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Figure S3. Packing diagram of **1** along the crystallographic *c*-axis. The *a*- and the *b*-axes are shown in red and green, respectively.

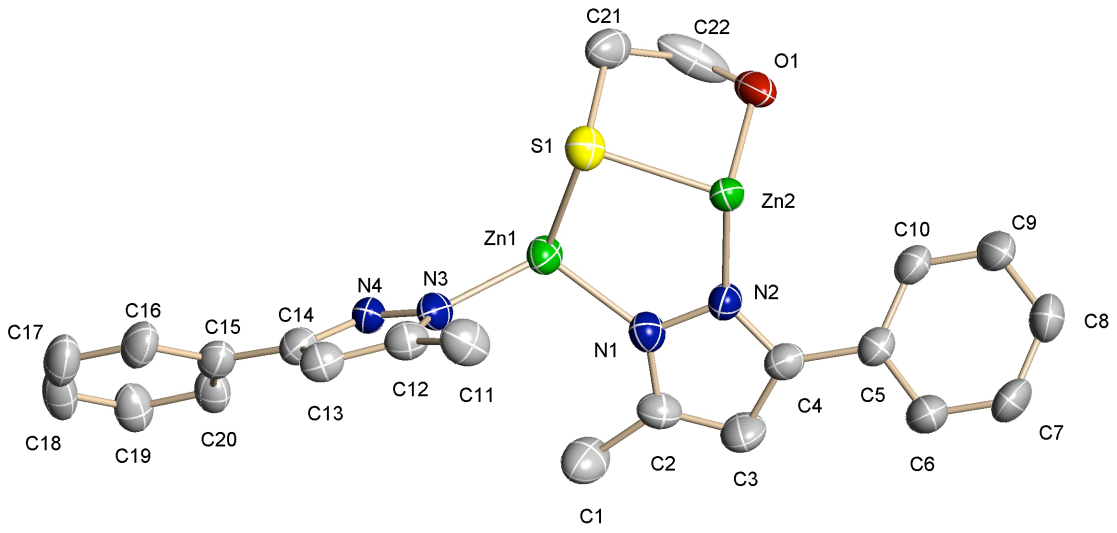
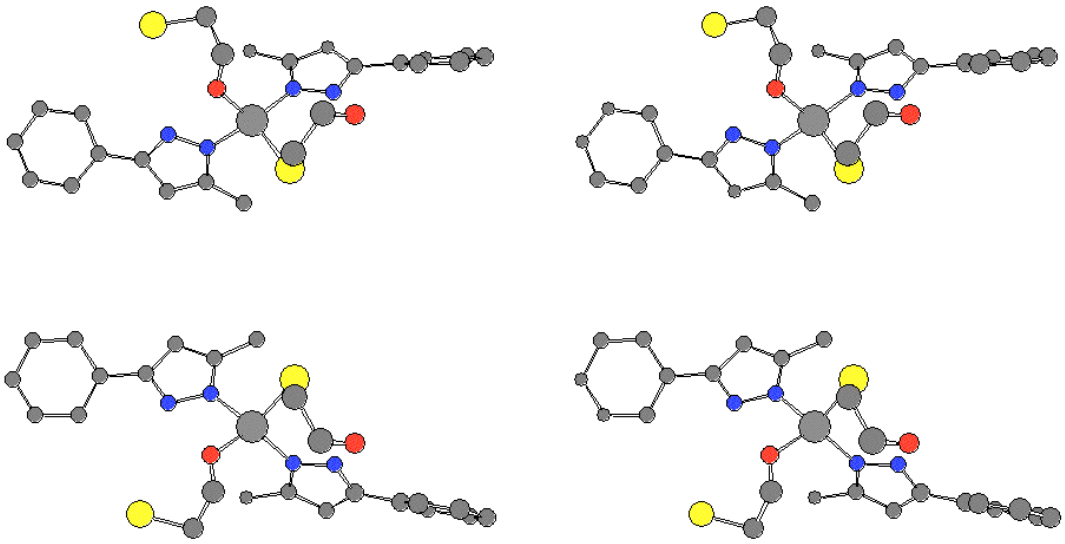


Figure S1. Diagram of the asymmetric unit for **1** (ORTEP, 50% probability ellipsoids). Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°) for compound **1**: Zn(1)-N(1) 1.995(5), Zn(1)-N(3) 2.006(5), Zn(1)-O(1) 1.970(5), Zn(1)-S(1) 2.3319(17), Zn(2)-N(2) 1.971(5), Zn(2)-N(4) 1.962(5), Zn(2)-O(1) 1.988(5), Zn(2)-S(1) 2.3240(17), N(1)-Zn(1)-N(3) 116.52(19), O(1)-Zn(1)-N(1) 116.32(19), O(1)-Zn(1)-N(3) 97.09(19), O(1)-Zn(1)-S(1) 111.82(14), N(1)-Zn(1)-S(1) 105.14(14), N(3)-Zn(1)-S(1) 109.99(14), N(4)-Zn(2)-N(2) 119.06(18), N(2)-Zn(2)-O(1) 113.82(19), N(4)-Zn(2)-O(1) 98.9(2), N(4)-Zn(2)-S(1) 124.02(14), N(2)-Zn(2)-S(1) 106.58(14), O(1)-Zn(2)-S(1) 89.99(13). Note that Zn(1) binds to a symmetry equivalent atom of O(1) and Zn(2) binds to a symmetry equivalent atom of N(4).



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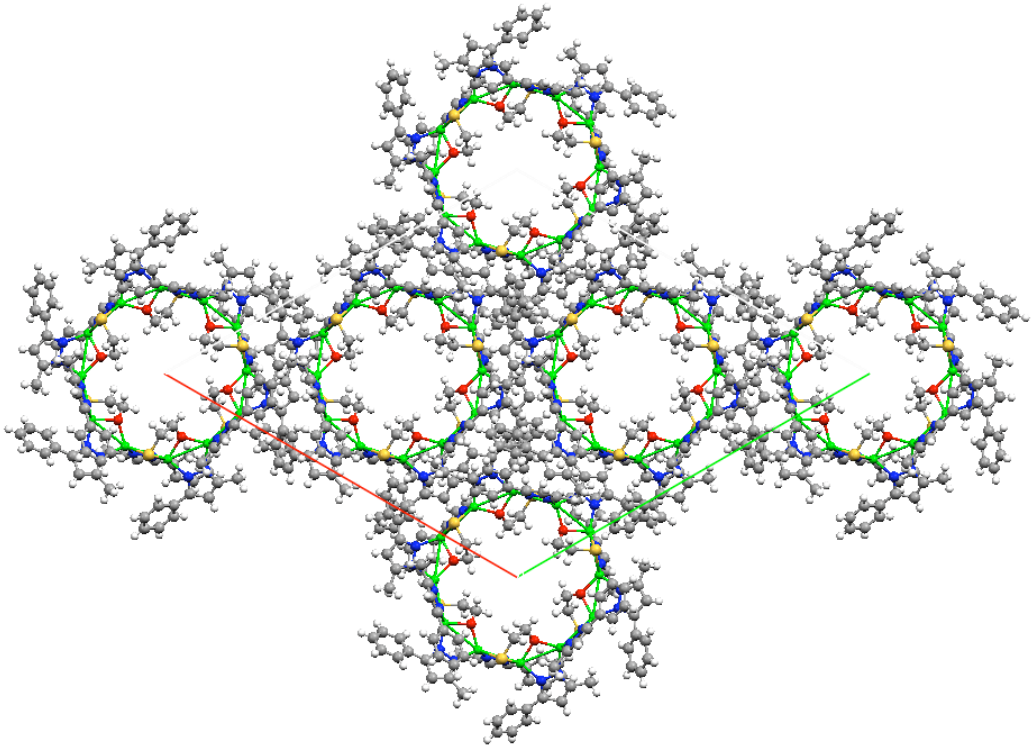

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