Electronic Supplementary Information

Cocrystallization of racemic amino acids with $ZnCl_2$: an investigation of chiral selectivity upon coordination to the metal centre.

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Content

S1. Structural data

Table S-1. Crystal data and details of measurements for all the complexes described in this work.

	***rac*-Isoleucine$_2$ ·ZnCl$_2$**	***meso*-Proline$_2$ ·ZnCl$_2$**	***rac*-Serine$_2$ ·ZnCl$_2$**	***meso*-Threonine$_2$ ·ZnCl$_2$ ·Threonine**	***catena*- [(μ_2-*DL*-Asparagine)ZnCl$_2$]**	***catena*-[(μ_2-*DL*-Tyrosine)ZnCl$_2$]**	***rac*-Proline$_2$ ·ZnCl$_2$**	***rac*-Proline$_2$ ·ZnBr$_2$**
Chemical formula	$C_{12}H_{26}Cl_2N_2O_4Zn$	$C_{10}H_{18}Cl_2N_2O_4Zn$	$C_6H_{13}Cl_2N_2O_6Zn$	$C_8H_{18}Cl_2N_2O_6Zn \cdot C_4H_9NO_3$	$C_4H_8Cl_2N_2O_3Zn$	$C_9H_{11}Cl_2NO_3Zn$	$C_{10}H_{18}Cl_2N_2O_4Zn$	$C_{10}H_{18}Br_2N_2O_4Zn$
M_r, g mol^{-1}	394.62	366.53	345.45	493.63	268.39	317.46	366.53	455.45
T / K	293 (2)	293 (2)	293 (2)	293 (2)	293 (2)	293 (2)	293 (2)	293 (2)
Crystal system	Triclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	*P*-1	$P2_1/c$	$P2_1/c$	*P*-1	$P2_1/c$	$P2_1/n$	*C2/c*	*C2/c*
a / Å	6.1647 (4)	8.7133 (3)	10.1190 (4)	9.2147 (5)	10.0109 (19)	8.8022 (10)	18.7127 (13)	18.6238 (11)
b / Å	12.6246 (7)	6.6937 (3)	13.5305 (7)	9.3042 (5)	6.8396 (8)	17.1083 (15)	5.9481 (6)	5.9591 (4)
c / Å	13.4501(8)	25.1323 (9)	8.9330 (4)	12.7858 (8)	13.3557 (16)	8.8138 (8)	13.6392 (11)	14.4189 (9)
α / °	62.666 (6)	90	90	110.722 (6)	90	90	90	90
β / °	84.162 (5)	94.159 (3)°	91.634 (4)	103.789 (5)	107.375 (15)	116.611 (13)	104.335 (8)	104.296 (6)
γ / °	89.311 (5)	90	90	90.346 (5)	90	90	90	90
V / Å^3	924.37 (11)	1461.96 (10)	1222.57 (10)	990.79 (11)	872.7 (2)	1186.7 (2)	1470.8 (2)	1550.67 (17)
Z, Z'	2, 1	4, 1	4, 1	2, 1	4, 1	4, 1	4, 0.5	4, 0.5
d / mg cm^{-3}	1.418	1.665	1.877	1.655	2.043	1.777	1.655	1.951
μ / mm^{-1}	1.63	2.06	2.46	1.56	3.39	2.51	2.04	6.75
Measd reflns	7348	6952	5665	8166	3851	5109	3307	3594
Indep reflns	4238	3369	2773	4576	1995	2729	1711	1799
Reflns with $I > 2\sigma(I)$	3308	2819	2100	3479	1371	1292	1139	1346
R_{int}	0.028	0.040	0.047	0.037	0.047	0.080	0.046	0.025
***R*[$F^2 > 2\sigma(F^2)$]**	0.050	0.045	0.058	0.048	0.067	0.072	0.064	0.044
***wR*(F^2)**	0.124	0.099	0.140	0.146	0.189	0.203	0.164	0.107

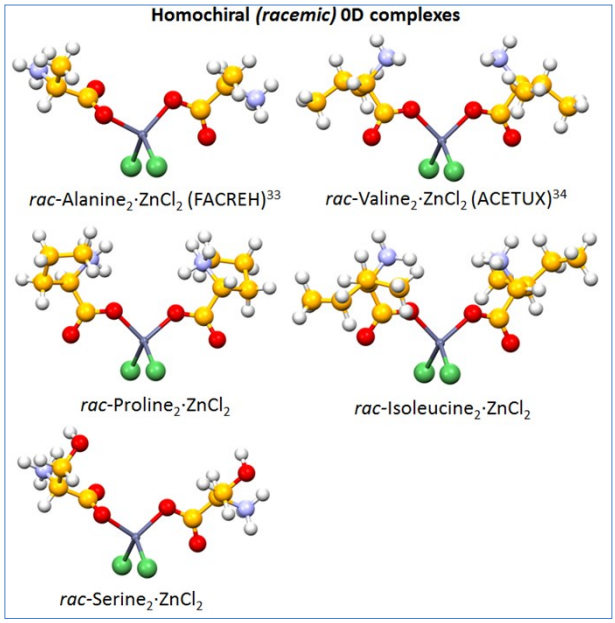

Figure S-1. Homochiral complexation: the crystals contain complexes of DD and LL in racemic mixture. No conglomerate formation is observed.

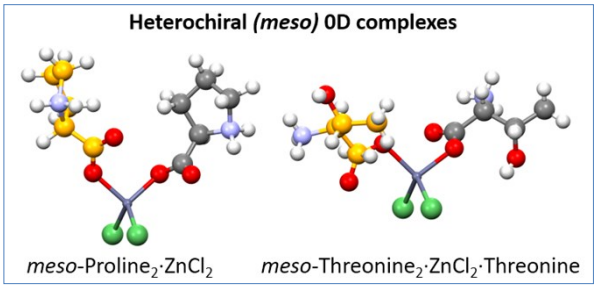

Figure S-2. Heterochiral complexes, which crystallize in *meso*-form.

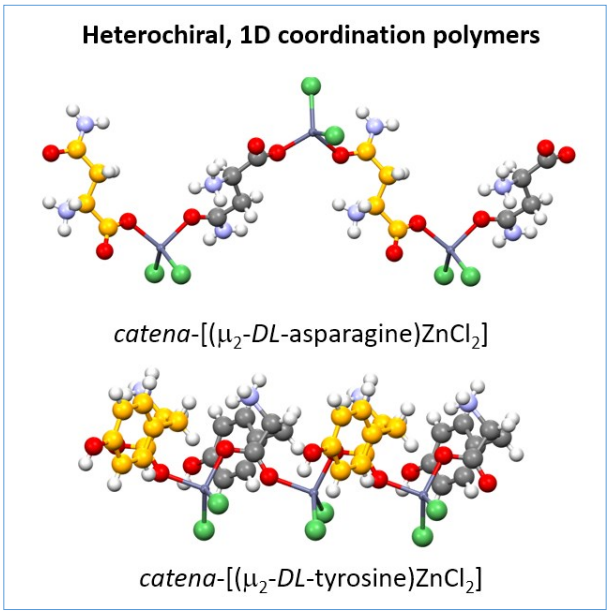

Figure S-3. The 1D polymers in *catena*-[(μ_2-*DL*-asparagine)$ZnCl_2$] and *catena*-[(μ_2-*DL*-tyrosine)$ZnCl_2$]: the chains contain alternating D and L amino acids.

S2. XRPD

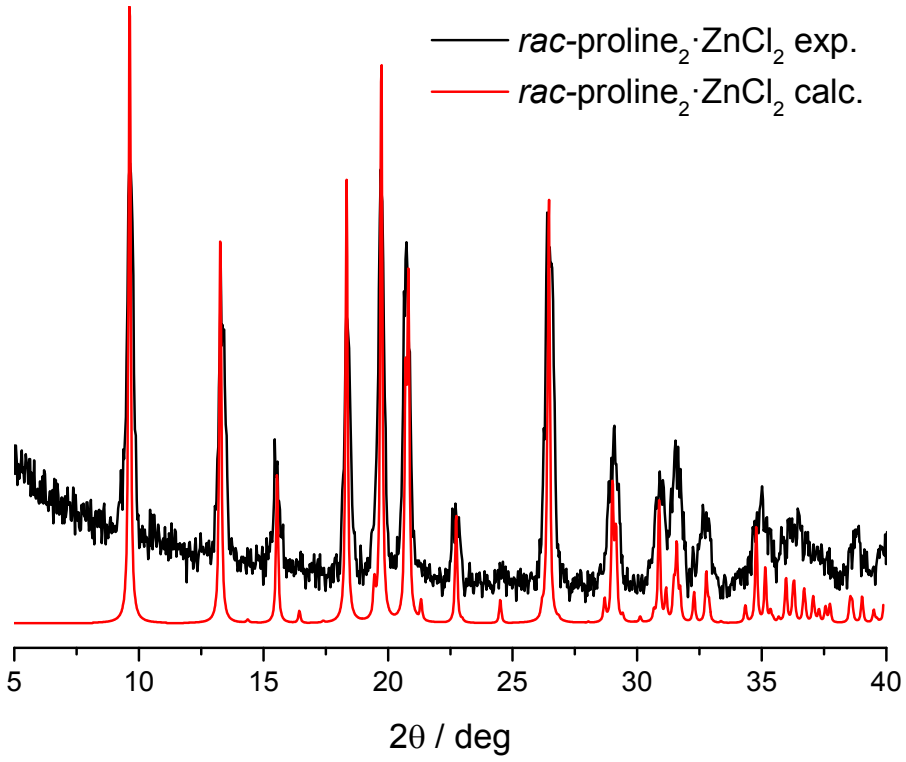

Fig. S-4. Comparison of (top, black line) the room temperature experimental XRPD patterns for *rac*-proline$_2$·ZnCl$_2$, obtained by slurry experiment in EtOH, and (bottom, red line) the pattern calculated on the basis of single crystal data.

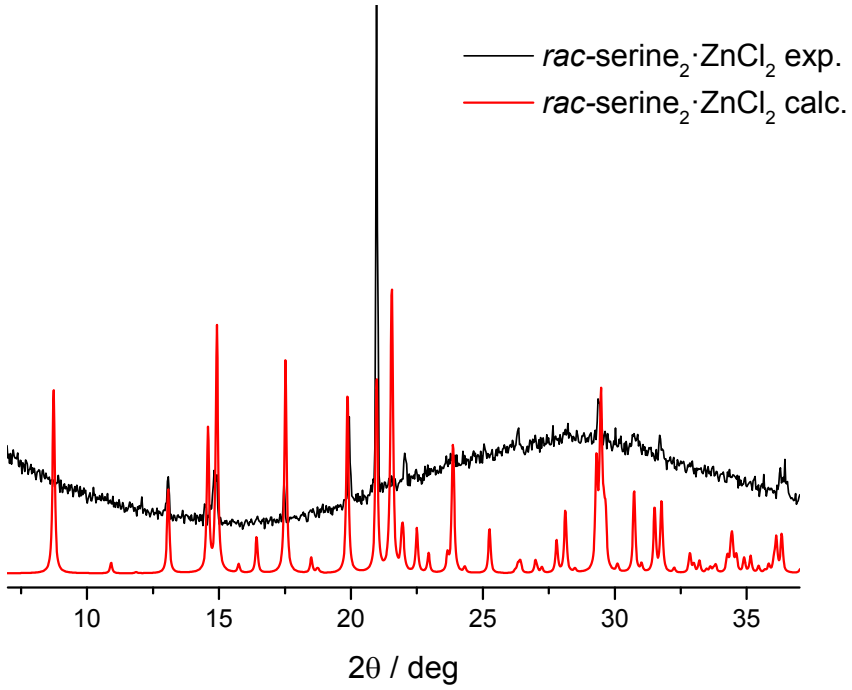

Fig. S-5. Comparison of the experimental (black line) and calculated (red line) XRPD patterns for *rac*-serine$_2$·ZnCl$_2$.

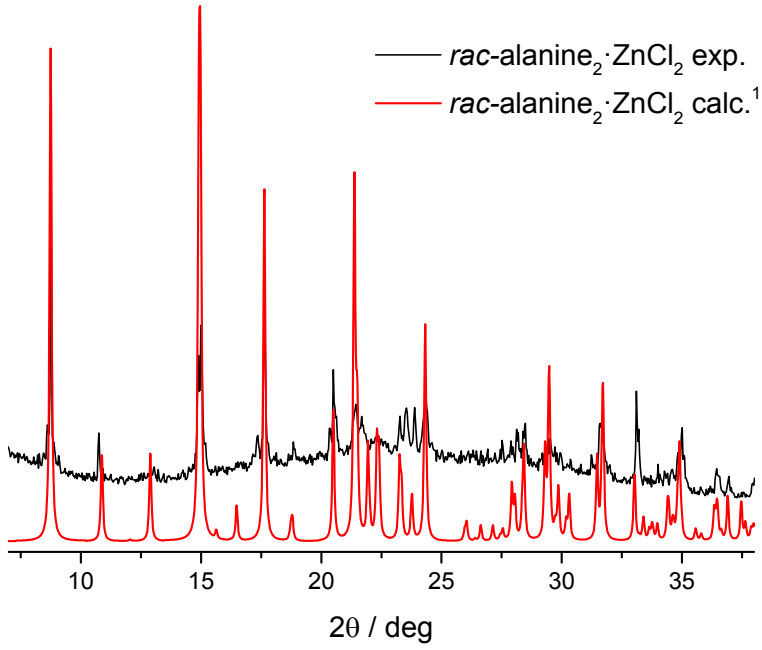

Fig. S-6. Comparison of the experimental (black line) and calculated (red line) XRPD patterns for *rac*-alanine$_2$·ZnCl$_2$ [refcode FACREH[1]].

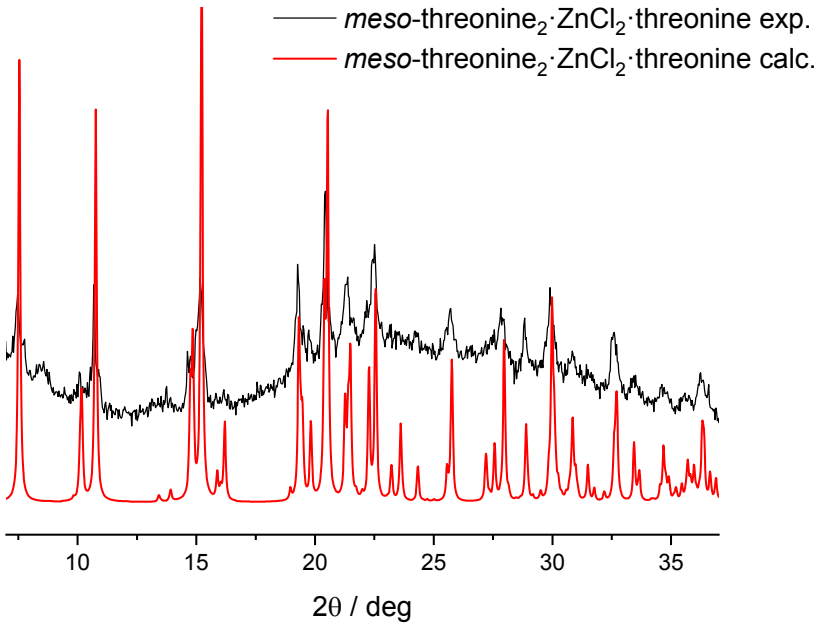

Fig. S-7. Comparison of the experimental (black line) and calculated (red line) XRPD patterns for *meso*-threonine$_2$·ZnCl$_2$·threonine.

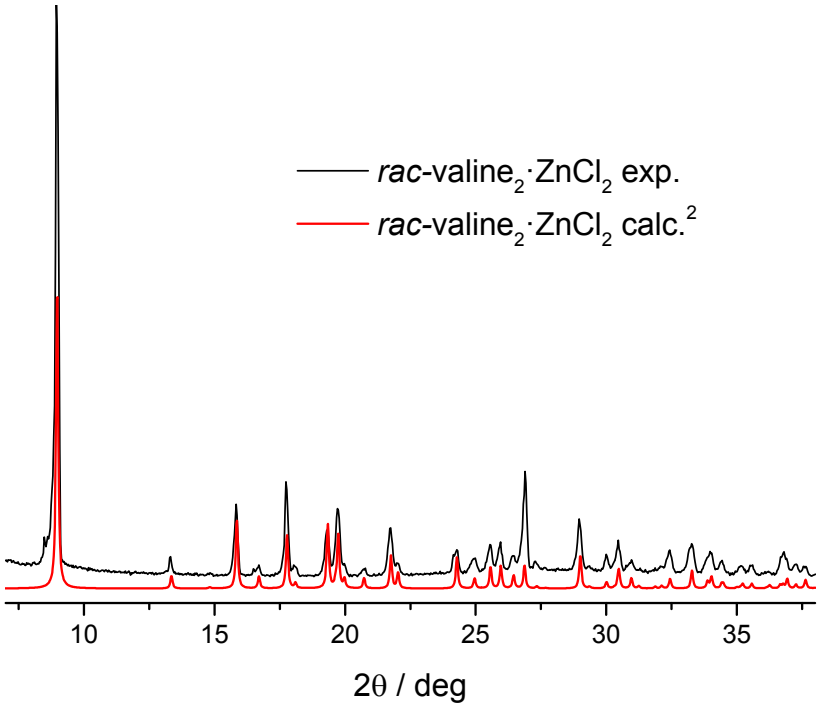

Fig. S-8. Comparison of the experimental (black line) and calculated (red line) XRPD patterns for *rac*-valine$_2$·ZnCl$_2$ [refcode ACETUX[2]].

References:

1. M. Subha Nandhini, R. V. Krishnakumar and S. Natarajan, *Acta Crystallogr. Sect. E: Struct. Rep. Online*, 2002, **58**, m127-m129.

2. M. S. Nandhini, R. V. Krishnakumar and S. Natarajan, *Acta Crystallogr. Sect. E: Struct. Rep. Online*, 2001, **57**, M498-M500.