

对称性破缺：手性高氯酸乙酸·二(乙二胺)合锌(II)的合成与结构

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Symmetry Breaking: Synthesis、Crystal Structure of Chiral Acetatobis(diaminoethane)zinc(II) Perchlorate

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Table S1. The crystallographic data of complexes

Number	1	2	3	4	5	6
formula	C ₆ H ₁₉ N ₄ ZnClO ₆	C ₆ H ₁₉ N ₄ ZnClO ₆	C ₆ H ₁₉ N ₄ ZnClO ₆	C ₆ H ₁₉ N ₄ ZnClO ₆	C ₆ H ₁₉ N ₄ ZnClO ₆	C ₆ H ₁₉ N ₄ ZnClO ₆
fw	344.07	344.07	344.07	344.07	344.07	344.07
temperature (K)	296(2)	296(2)	296(2)	296(2)	296(2)	296(2)
crystal size (mm)	0.36 × 0.32 × 0.18	0.46 × 0.36 × 0.17	0.42 × 0.36 × 0.18	0.45 × 0.38 × 0.22	0.47 × 0.42 × 0.19	0.45 × 0.40 × 0.21
crystal system	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal	Tetragonal
space group	<i>P</i> 4 ₃ 2 ₁ 2	<i>P</i> 4 ₃ 2 ₁ 2	<i>P</i> 4 ₃ 2 ₁ 2	<i>P</i> 4 ₁ 2 ₁ 2	<i>P</i> 4 ₃ 2 ₁ 2	<i>P</i> 4 ₃ 2 ₁ 2
<i>a</i> / Å	9.5807(3)	9.5889(10)	9.5900(10)	9.5907(10)	9.5930(2)	9.5856(2)
<i>b</i> / Å	9.5807(3)	9.5889(10)	9.5900(10)	9.5907(10)	9.5930(2)	9.5856(2)
<i>c</i> / Å	30.7645(19)	30.8098(6)	30.8075(6)	30.8097(6)	30.8173(10)	30.7979(9)
volume / Å ³	2823.9(2)	2832.87(7)	2833.31(7)	2833.92(7)	2835.98(12)	2829.83(12)
<i>Z</i>	8	8	8	8	8	8
<i>D_c</i> /g cm ⁻³	1.619	1.613	1.613	1.613	1.612	1.615
<i>μ</i> / mm ⁻¹	1.953	1.946	1.946	1.946	1.944	1.948
<i>F</i> (000)	1424	1424	1424	1424	1424	1424
unique refl. (<i>R</i> _{int})	3223 (0.0206)	3233(0.0226)	3283 (0.0257)	3236(0.0235)	3221 (0.0208)	3243 (0.0221)
<i>S</i> on <i>F</i> ²	1.088	1.062	1.074	1.050	1.079	1.010
<i>R</i> ₁ , ^{<i>a</i>} <i>wR</i> ₂ ^{<i>b</i>} (<i>I</i> > 2σ (<i>I</i>))	0.0504, 0.1363	0.0522, 0.1422	0.0579, 0.1467	0.0471, 0.1337	0.0547, 0.1449	0.0469, 0.1387
<i>R</i> ₁ , ^{<i>a</i>} <i>wR</i> ₂ ^{<i>b</i>} (all data)	0.0586, 0.1430	0.0617, 0.1546	0.0733, 0.1623	0.0515, 0.1366	0.0659, 0.1623	0.0526, 0.1497
Absolute structure parameter	0.03(3)	0.04(3)	0.04(3)	0.01(3)	0.01(3)	0.03(3)

