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cis-[Ni(NCS)$_2$tren]的镜面对称性破缺：螯环的特殊手性构象

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Mirror Symmetry Breaking of *cis*-[Ni(NCS)$_2$tren]: Special Chiral Conformations of Chelate Rings

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Table S1　*cis*-[Ni(NCS)$_2$(tren)]的晶体学数据和精修结果

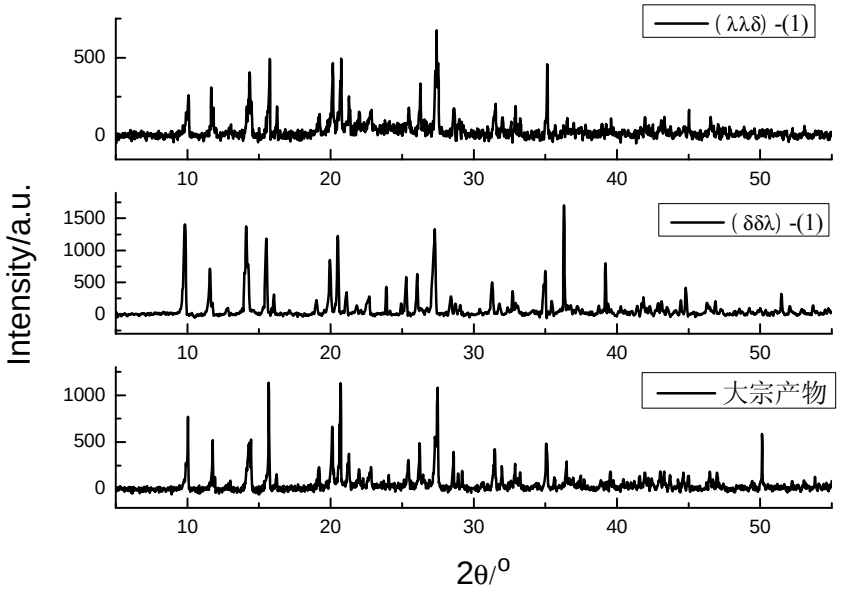
Table S1　Crystallographic and structural refinement parameters for *cis*-[Ni(NCS)$_2$(tren)]

Empirical formula	$C_8H_{18}N_6S_2Ni$ (λλδ)	$C_8H_{18}N_6S_2Ni$ (δδλ)	$C_8H_{18}N_6S_2Ni$ (δδλ)[7]
Formula weight	321.11	321.11	321.11
Crystal shape/Crystal colour	block / Light blue	block / Light blue	Block / Light blue
Temperature	**173(2) K**	**173(2) K**	**298(2) K**
Wavelength	0.071073 nm	0.071073 nm	0.071073 nm
Crystal system, Space group	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$	Orthorhombic, $P2_12_12_1$
Unit cell dimensions	a = 0.85026(15) nm	a = 0.85640(13) nm	a = 0.8646(4) nm
	b = 1.0754(2) nm	b = 1.08133(2) nm	b = 1.0852(5) nm
	c = 1.4591(3) nm	c = 1.4654(3) nm	c = 1.4704(7) nm
Volume	1.3342(4) nm^3	1.3570(4) nm^3	1.3797(4) nm^3
Z, Calculated density	4, **1.599** mg·cm^{-3}	4, **1.572** mg·cm^{-3}	4, **1.546** mg·cm^{-3}
Absorption coefficient	None	None	None
F (000)	672	672	672
range for data collection	2.35 to 26.00°	2.35 to 26.00°	2.33 to 26.05°
Limiting indices	$-6 \le h \le 10$, $-13 \le k \le 11$, $-17 \le$	$-10 \le h \le 10$, $-13 \le k \le 9$, $-18 \le$	$-10 \le h \le 10$, $-13 \le k \le 13$, $-18 \le l$
	$l \le 13$	$l \le 17$	≤ 17
Reflections collected	6786	7198	10627
Independent reflections	2588 [R(int) = 0.0353]	2610 [R(int) = 0.0207]	2506 [R(int) = 0.0299]
Completeness to = 26.00°	99.3%	99.3%	99.3%
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	2588 / 0 / 154	2610 / 0 / 154	2506 / 0 / 154
Goodness-of-fit on F^2	1.070	1.057	0.956
Final R indices [$I > 2$ (I)]	R_1 = 0.0295, wR_2 = 0.0717	R_1 = 0.0212, wR_2 = 0.0512	R_1 = 0.0250, wR_2 = 0.0613
R indices (all data)	R_1 = 0.0303, wR_2 = 0.0722	R_1 = 0.0216, wR_2 = 0.0515	R_1 = 0.0694, wR_2 = 0.1101
Absolute structure parameter	0.019(14)	0.018(11)	0.03(2)
Largest diff. peak and hole	0.882 and -0.517 e. Å^{-3}	0.263 and -0.212 e. Å^{-3}	1.044 and -1.542 e. Å^{-3}

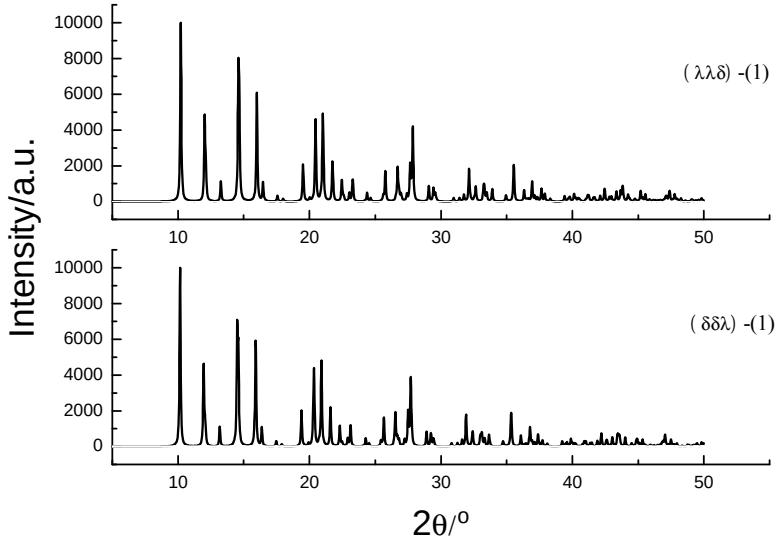
Table S2　(λλδ)-*cis*-[Ni(NCS)$_2$(tren)]的部分键长、键角

Table S2　Bond lengths [Å] and angles [deg] for (λλδ)-*cis*-[Ni(NCS)$_2$(tren)] (1)

C(1)-N(1)	1.485(3)	C(1)-C(2)	1.519(4)
C(2)-N(2)	1.476(3)	C(3)-N(1)	1.473(3)
C(3)-C(4)	1.507(4)	C(4)-N(3)	1.473(4)
C(5)-N(1)	1.467(3)	C(5)-C(6)	1.505(4)
C(6)-N(4)	1.476(4)	C(7)-N(5)	1.148(4)
C(7)-S(1)	1.632(3)	C(8)-N(6)	1.154(4)
C(8)-S(2)	1.637(3)	N(1)-Ni(1)	2.085(2)
N(2)-Ni(1)	2.077(2)	N(3)-Ni(1)	2.119(3)
N(4)-Ni(1)	2.135(2)	N(5)-Ni(1)	2.050(2)
N(6)-Ni(1)	2.086(2)		
N(1)-C(1)-C(2)	113.3(2)	N(2)-C(2)-C(1)	109.3(2)
N(1)-C(3)-C(4)	110.8(2)	N(3)-C(4)-C(3)	109.9(2)
N(1)-C(5)-C(6)	110.1(2)	N(4)-C(6)-C(5)	110.2(2)
N(5)-C(7)-S(1)	179.4(3)	N(6)-C(8)-S(2)	176.5(3)
C(5)-N(1)-C(3)	111.9(2)	C(5)-N(1)-C(1)	112.7(2)
C(3)-N(1)-C(1)	111.0(2)	C(5)-N(1)-Ni(1)	105.65(16)
C(3)-N(1)-Ni(1)	105.90(16)	C(1)-N(1)-Ni(1)	109.36(15)
C(2)-N(2)-Ni(1)	108.66(16)	C(4)-N(3)-Ni(1)	109.42(18)
C(6)-N(4)-Ni(1)	110.17(18)	C(7)-N(5)-Ni(1)	163.9(2)
C(8)-N(6)-Ni(1)	159.5(2)	N(5)-Ni(1)-N(2)	89.00(9)
N(5)-Ni(1)-N(1)	172.67(9)	N(2)-Ni(1)-N(1)	83.75(9)
N(5)-Ni(1)-N(6)	91.17(9)	N(2)-Ni(1)-N(6)	177.97(10)
N(1)-Ni(1)-N(6)	96.05(8)	N(5)-Ni(1)-N(3)	98.68(10)
N(2)-Ni(1)-N(3)	94.93(9)	N(1)-Ni(1)-N(3)	83.04(9)
N(6)-Ni(1)-N(3)	87.05(9)	N(5)-Ni(1)-N(4)	97.63(9)
N(2)-Ni(1)-N(4)	90.68(9)	N(1)-Ni(1)-N(4)	81.46(9)
N(6)-Ni(1)-N(4)	87.29(9)	N(3)-Ni(1)-N(4)	162.83(9)



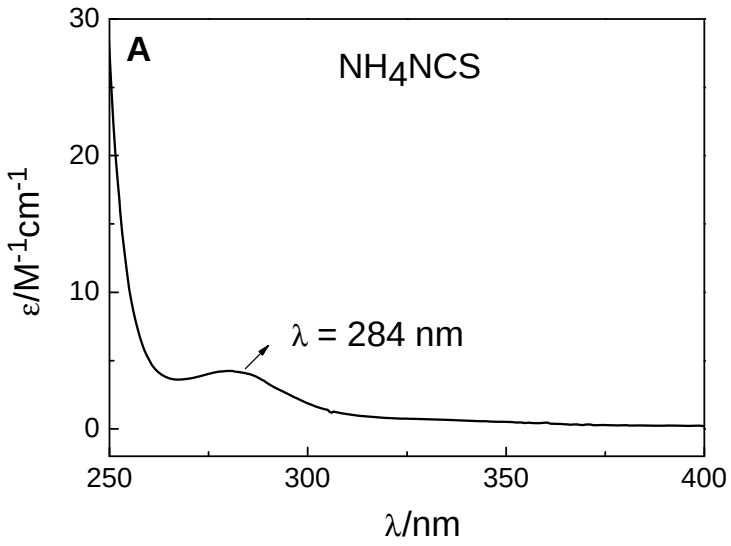
实验谱图(Experiment results)



模拟谱图(Data-fitting results)

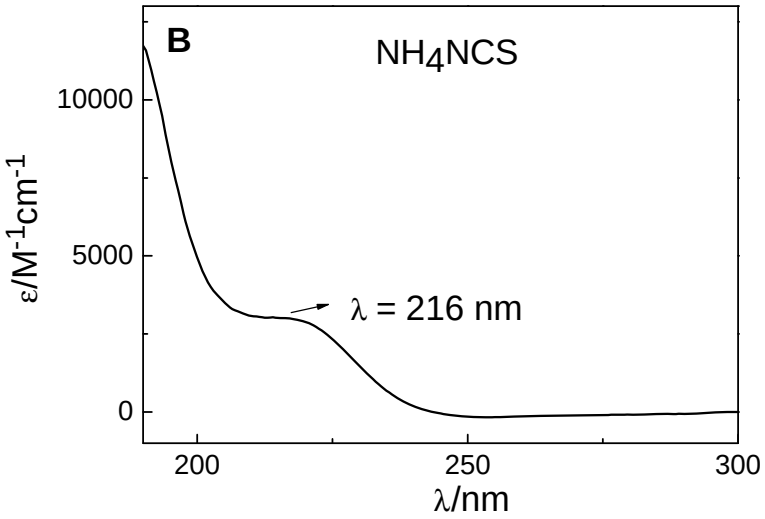
Fig.S3　(λλδ)-*cis*-[Ni(NCS)$_2$tren]和(δδλ)-*cis*-[Ni(NCS)$_2$tren]的单晶、大宗粉末和晶体数据拟合 XRD 谱图

Fig.S3　XRD spectra of single-crystal, bulk powder and data-fitting results for (λλδ)-*cis*-[Ni(NCS)$_2$tren] and (δδλ)-*cis*-[Ni(NCS)$_2$tren]



(A) NH_4NCS 水溶液的浓度为 3.4×10^{-2} mol·L^{-1}

(A) The concentration of NH_4NCS in H_2O is 3.4×10^{-2} mol·L^{-1}.

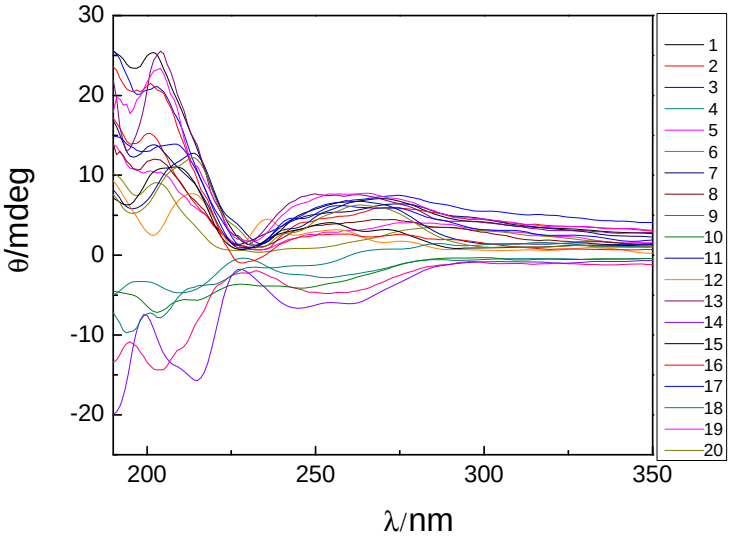


(B) NH_4NCS 水溶液的浓度为 1.425×10^{-4} mol·L^{-1}

(B) The concentration of NH_4NCS in H_2O is 1.425×10^{-4} mol·L^{-1}.

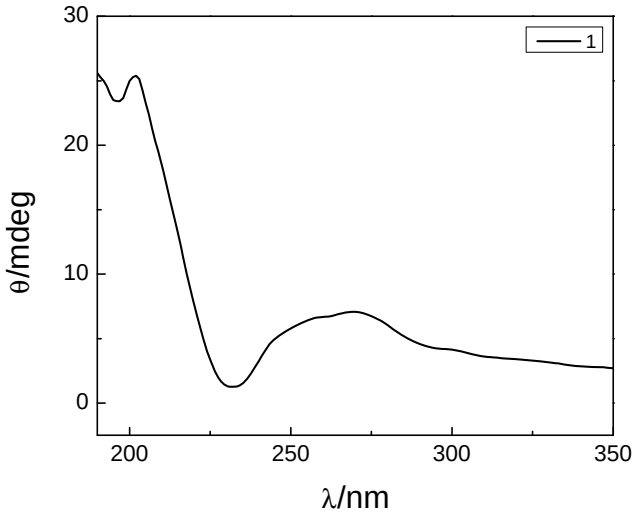
Fig.S4　NH_4NCS 的溶液 UV 谱图.

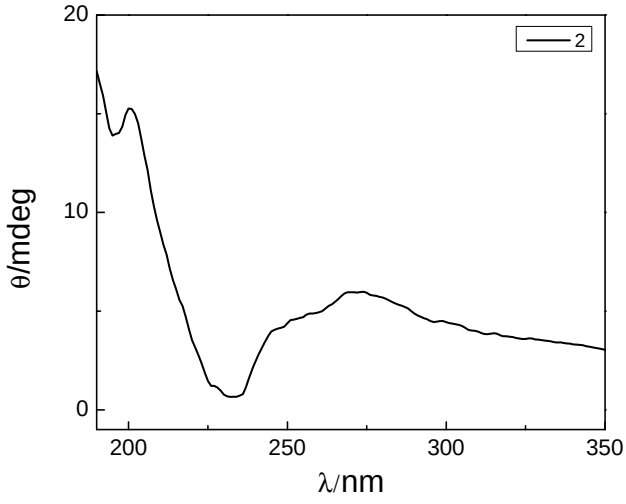
Fig.S4　UV-spectrum of NH_4NCS solution

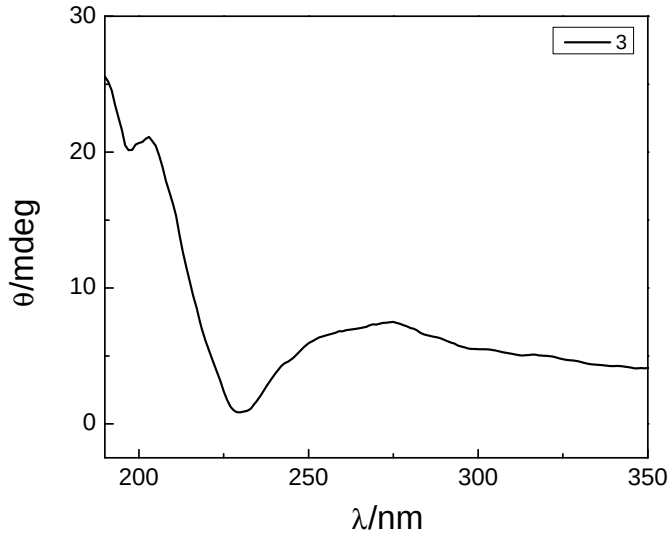


20次平行实验大宗产物的固体CD叠加图

Solid-state CD overlay-spectra of *cis*-[Ni(NCS)$_2$tren] from twenty batch syntheses



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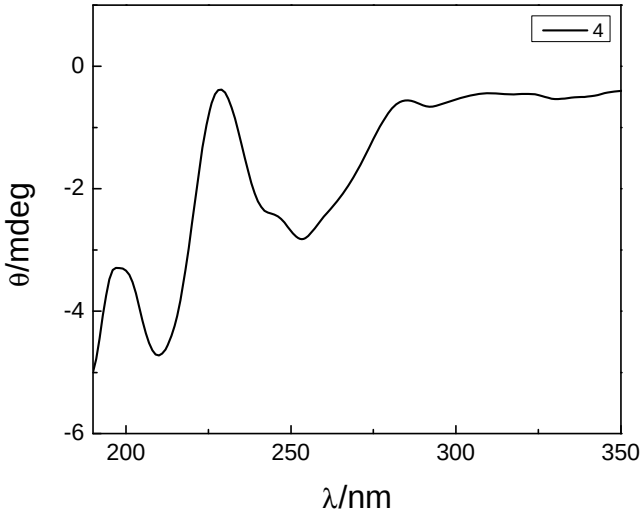
10
0
θ/mdeg
200
250
300
350
λ/nm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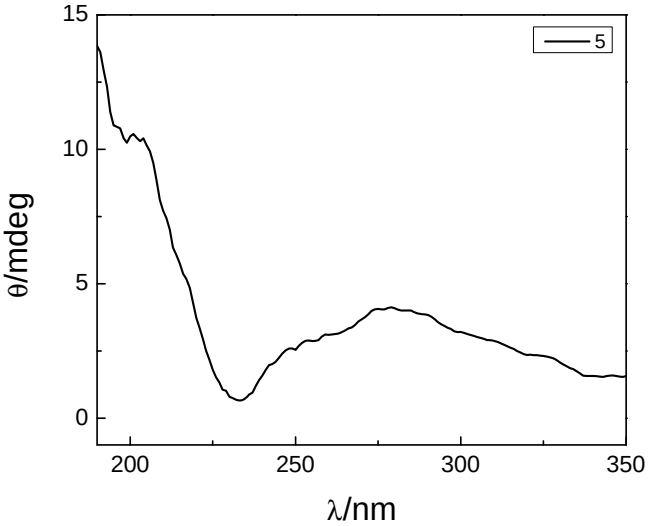
λ/nm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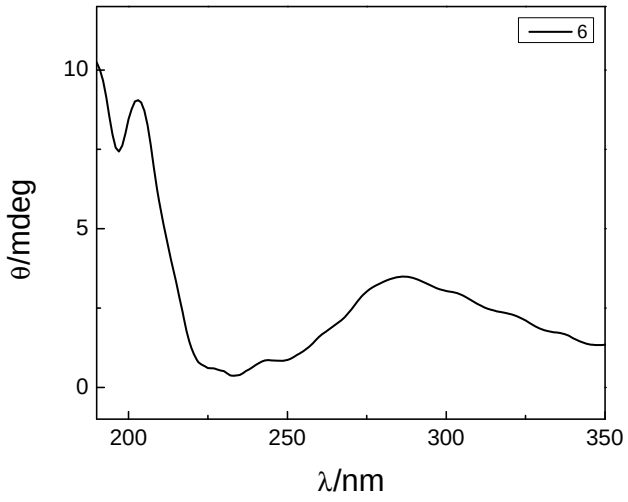
5
0
θ/mdeg
200
250
300
350
λ/nm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λ/nm
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10
200
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300
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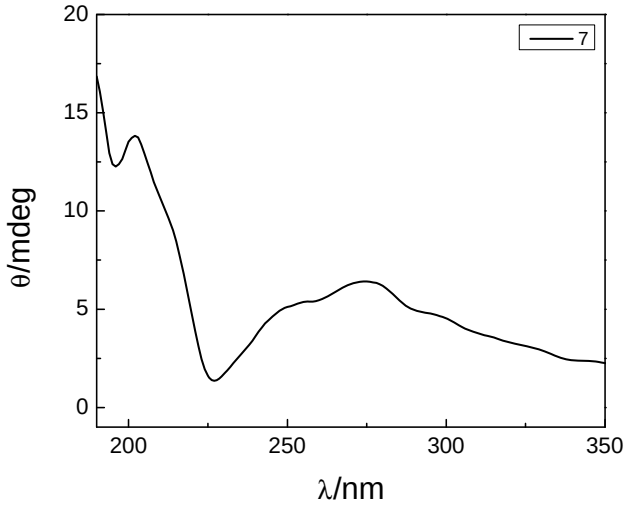
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λ/nm
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10
15
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200
250
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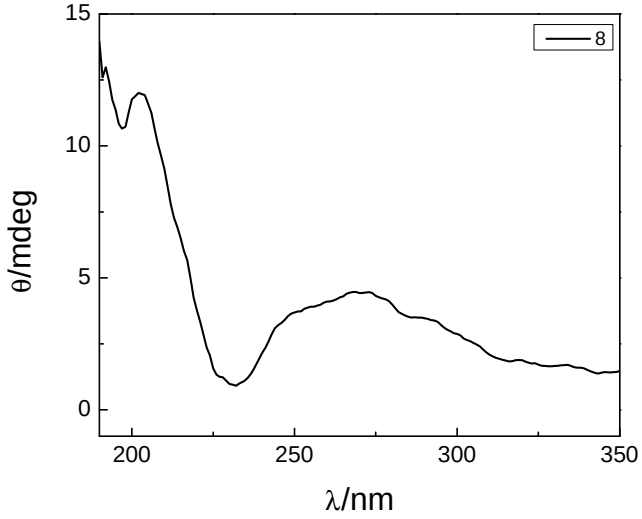
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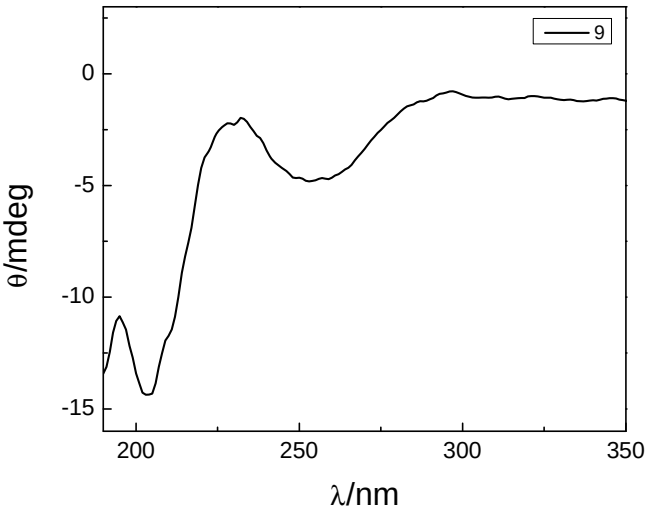
θ/mdeg
λ/nm
0
5
10
15
200
250
300
350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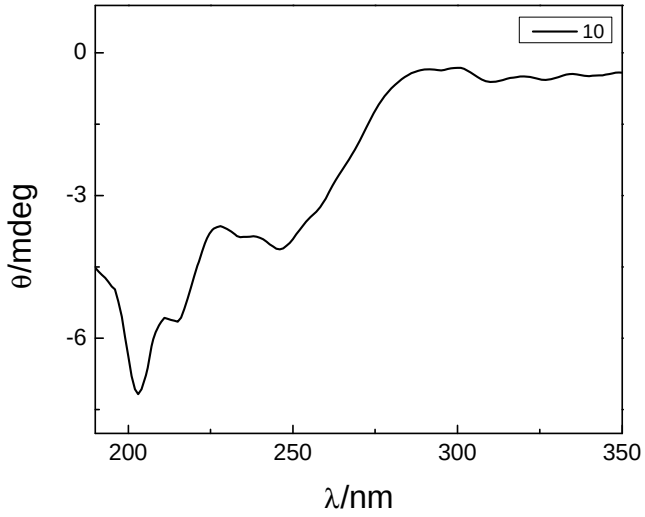
θ/mdeg
200
250
300
350
λ/nm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θ/mdeg
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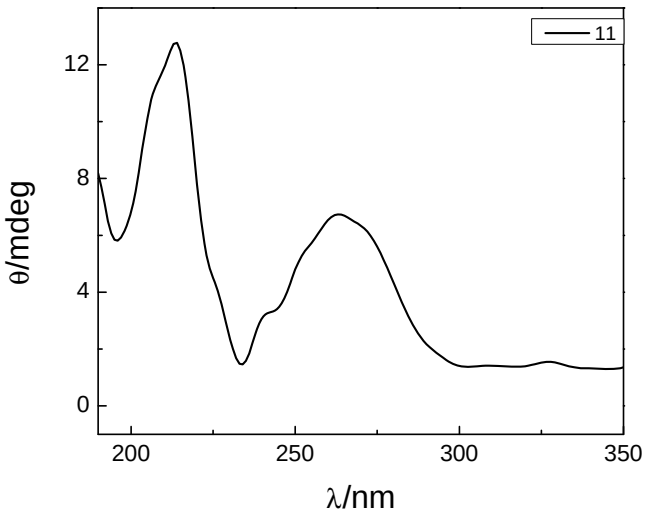
λ/nm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0
θ/mdeg
200
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300
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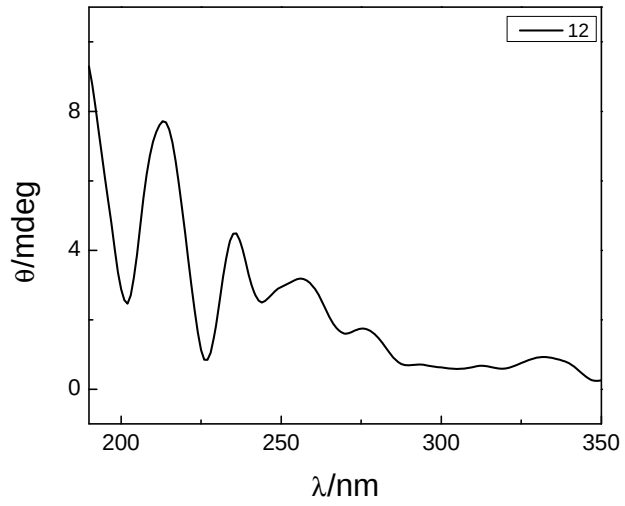
λ/nm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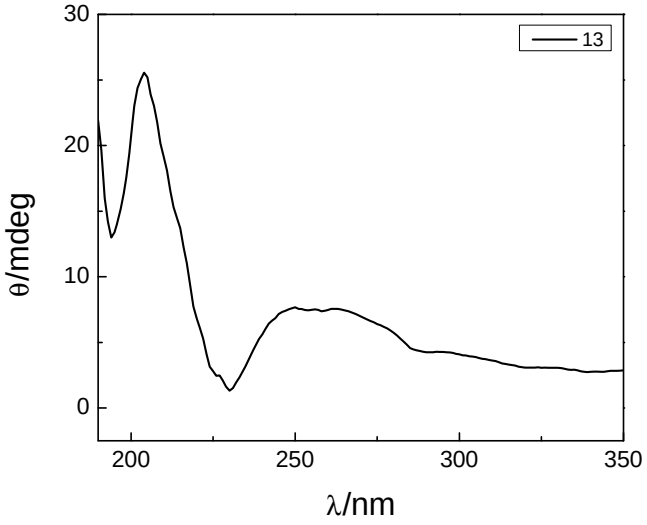
λ/nm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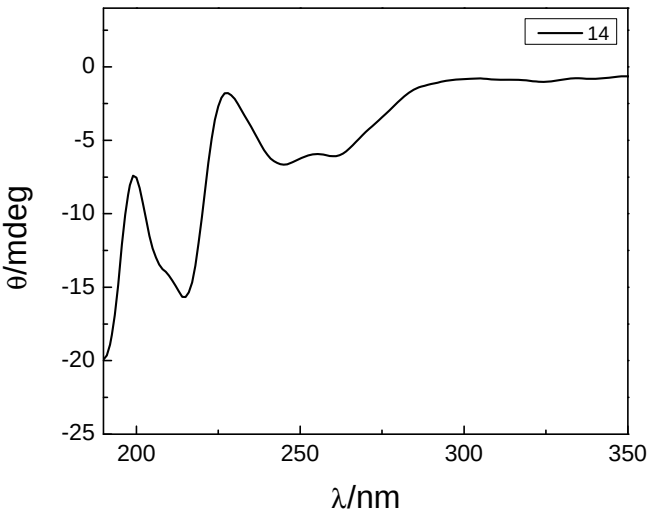
λ/nm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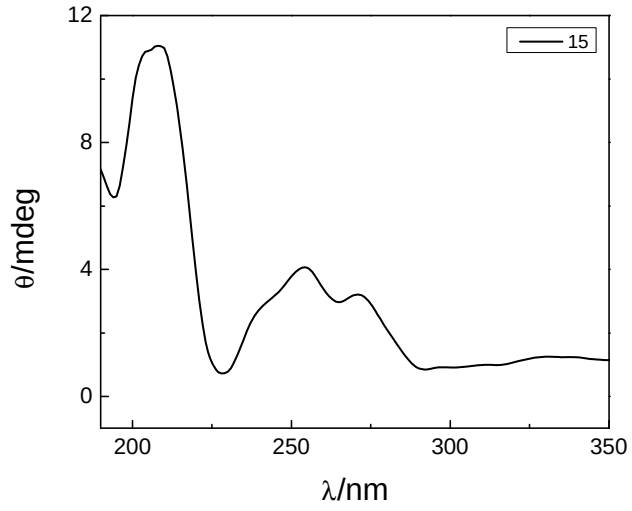
250
300
350
λ/nm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θ/mdeg
λ/nm
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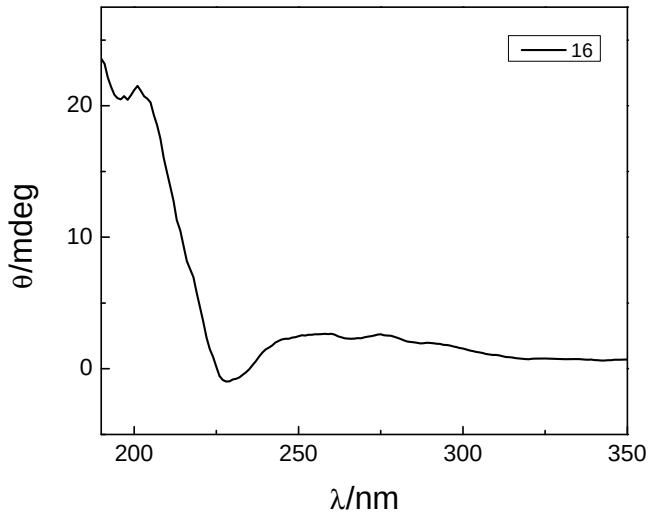
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λ/nm
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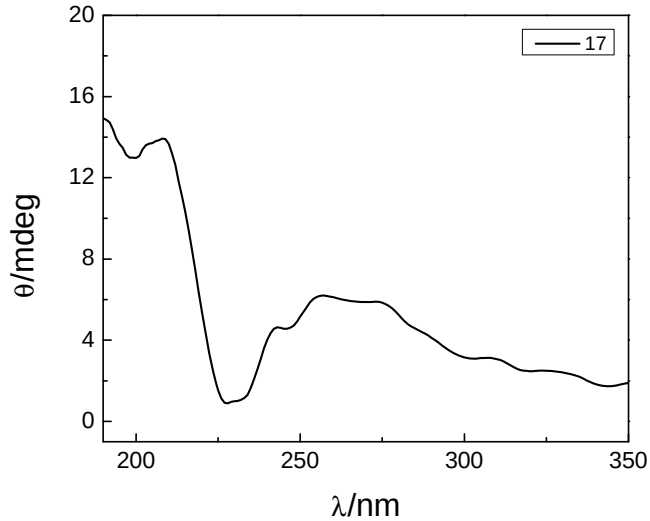
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λ/nm
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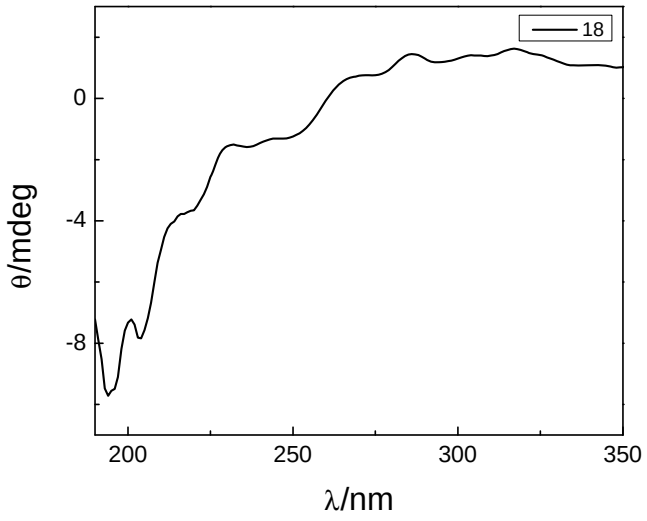

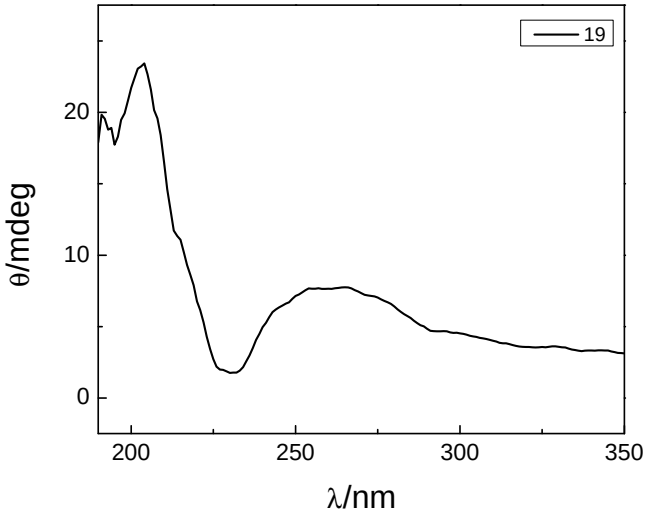

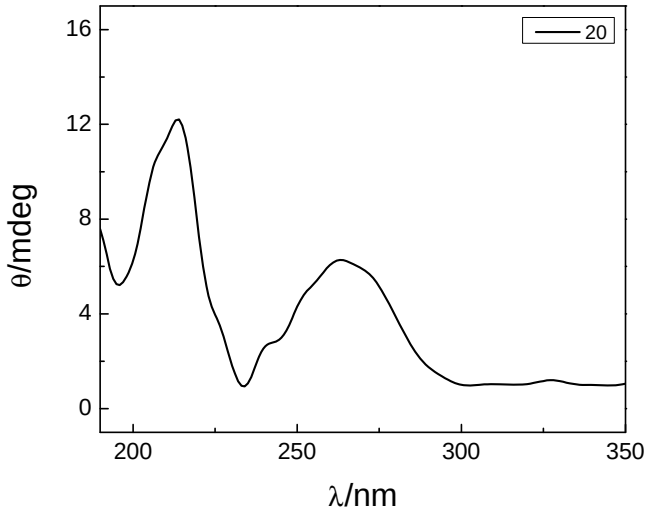

Fig.S5　20个批次合成实验的大宗产物固体CD光谱

Fig.S5 Solid-state CD spectra of *cis*-[Ni(NCS)$_2$tren] from twenty batch syntheses