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Influence of the counterion in the supramolecular frameworks of isoquinoline-based silver(I) complexes

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Supporting Information

ÍNDICE

Table S1. Selected bond distances (Å) and angles (°) for compounds **2** - **9**

2[a]	Ag1–N2	2.152(5)	N2–Ag1–N2a	177.9(2)
3[b]	Ag1–N2	2.246(3)	N2–Ag1–O3	96.45(11)
	Ag1–N4	2.247(3)	N2–Ag1–O3a	91.96(10)
	Ag1–O3	2.429(3)	N4–Ag1–O3	104.77(11)
	Ag1–O3a	2.706(2)	N4–Ag1–O3a	99.69(9)
	N2–Ag1–N4	158.15(12)	O3–Ag1–O3a	71.13(9)
4[c]	Ag1–N2	2.197(3)	N2–Ag1–N4	156.72(10)
	Ag1–N4	2.193(3)	N2–Ag1–O2a	101.12(10)
	Ag1–O2a	2.513(2)	N4–Ag1–O2a	102.06(10)
5	Ag1–N2	2.169(2)	N2–Ag1–N4	158.61(8)
	Ag1–N4	2.187(2)		
6	Ag1–N2	2.156(4)	N2–Ag1–N4	164.11(13)
	Ag1–N4	2.153(4)	N2–Ag1–O1W	96.34(15)
	Ag1–O1W	2.534(4)	N4–Ag1–O1W	98.99(15)
8[d]	Ag1–N2	2.227(5)	N2–Ag1–N4a	167.48(17)
	Ag1–N4a	2.224(4)	N2–Ag1–O1W	94.01(17)
	Ag1–O1W	2.580(5)	N4a–Ag1–O1W	98.39(16)
9[e]	Ag1–N2	2.176(5)	N2a–Ag1–N4	171.3(2)
	Ag1–N4	2.166(5)	N2a–Ag1–O3a	95.1(4)
	Ag1–O3a	2.535(17)	N4–Ag1–O3a	93.6(4)

[a]Symmetry code for **2**: (a) = *-x+1, y, -z+1/2*.

[b]Symmetry code for **3**: (a) = *-x+1, -y+1, -z+1*.

[c]Symmetry code for **4**: (a) = *-x+1, -y+1, -z+2*.

[d]Symmetry code for **8**: (a) = *x+1, y, z*.

[e]Symmetry code for **9**: (a) = *x, y-1, z*.

Table S2. Structural details of the π-π interactions in compounds **2** - **9**

Compound	Isoquinoline groups[a]	Centroid-centroid (Å)	Off-set angle (°)	Symm[b]
2	N2···N2	4.265(5)	39.0(2)	-1
3	N2···N2	3.979(5)	22.3(4)	-1
	N2···N4	3.916(6)	21.7(6)	-
4	N2···N2	4.006(4)	31.7(3)	-1
	N2···N4	4.283(5)	33.5(5)	-
5	N2···N2	4.458(7)	42.8(9)	-1
6	N2···N2	3.620(7)	16.7(8)	-1
	N4···N4	3.689(7)	23.9(9)	-1
8	N2···N2	3.604(6)	13.9(8)	-1
	N2···N2	3.707(6)	23.1(6)	-1
	N4···N4	3.628(6)	20.9(7)	-1
	N4···N4	3.657(6)	17.9(6)	-1
9	N2···N2	3.709(4)	3.1(6)	-1
	N2···N2	3.672(5)	19.9(6)	-1
	N4···N4	3.627(5)	26.8(5)	b (1/4,y,z)

[a]Nitrogen atom from the interacting isoquinoline group

[b]Symmetry relating the two interacting isoquinoline groups. When no symmetry is given, the two isoquinoline groups are crystallographically distinct.

Table S3. Conformational Analysis of Hydrocarbons Bridge for Ag($\mathbf{L^1}$), Ag($\mathbf{L^2}$) and Ag($\mathbf{L^3}$) compounds.

Compound	Angles (º)		Conformation*	Compound	Angles (º)		Conformation
$\mathbf{L^1}$**	O1-C1-N1-C11	-8.0(6)	eclipsed (synperiplanar)	**1****	O1-C1-N1-C11	2.8(4)	eclipsed (synperiplanar)
	N1-C11-C11^a-N1^a	60.4(4)	anticlinal		C1-N1-C11-C12	-113.5(3)	anticlinal
	C1-N1-C11-C11^a	-98.9(4)	gauche (synclinal)		N1-C11-C12-N3	64.9(3)	gauche (synclinal)
					C11-C12-N3-C13	-107.9(3)	anticlinal
					C12-N3-C13-O2	2.4(4)	eclipsed (synperiplanar)
2	O1-C1-N1-C11A	2.7(9)	eclipsado (synperiplanar)	**3**	O1-C1-N1-C11	-0.3(2)	eclipsado (synperiplanar)
	C1-N1-C11A-C11Aa	-145.6(7)	anticlinal		C1-N1-C11-C12	146.7(1)	anticlinal
	N1-C11A-C11Aa-N1a	-64.9(8)	gauche (synclinal)		N1-C11-C12-N3	-58.7(5)	gauche (synclinal)
	C11A-C11Aa-N3a-C13a	145.6(9)	anticlinal		C11-C12-N3-C13	-146.5(5)	anticlinal
	C11Aa-N3a-C13a-O2a	2.7(9)	eclipsado (synperiplanar)		C12-N3-C14-O2	5.2(5)	eclipsado (synperiplanar)
4	O1-C1-N1-C12	5.4(7)	eclipsado (synperiplanar)	**5**	O1-C1-N1-C12	1.1(3)	eclipsado (synperiplanar)
	C1-N1-C12-C13	-103.9(5)	anticlinal		C1-N1-C12-C13	-110.5(2)	anticlinal
	N1-C12-C13-N3	66.0(5)	gauche (synclinal)		N1-C12-C13-N3	66.0(2)	gauche (synclinal)
	C12-C13-N3-C15	-104.1(5)	anticlinal		C12-C13-N3-C15	-107.8(2)	anticlinal
	C13-N3-C15-O2	4.0(4)	eclipsado (synperiplanar)		C13-N3-C15-O2	3.3(3)	eclipsado (synperiplanar)
6	O1-C1-N1-C12	-1.9(7)	eclipsado (synperiplanar)	**7****	O1-C1-N2-C11	2.3(7)	eclipsado (synperiplanar)
	C1-N1-C12-C13	107.7(5)	anticlinal		C1-N2-C11-C12	-94.0(5)	anticlinal
	N1-C12-C13-N3	-62.4(5)	gauche (synclinal)		N2-C11-C12-C13	-59.4(5)	gauche (synclinal)
	C12-C13-N3-C15	107.2(5)	anticlinal		C11-C12-C13-N3	-56.5(5)	gauche (synclinal)
	C13-N3-C15-O2	-6.4(7)	eclipsado (synperiplanar)		C12-C13-N3-C14	-99.5(5)	anticlinal
					C13-N3-C14-O2	6.9(7)	eclipsado (synperiplanar)
8	O1-C1-N1-C11	2.4(1)	eclipsado (synperiplanar)	**9**	O1-C1-N1-C11	0.3(5)	eclipsado (synperiplanar)
	C1-N1-C11-C12	94.5(1)	anticlinal		C1-N1-C11-C12	93.2(4)	anticlinal
	N1-C11-C12-C13	41.0(1)	gauche (synclinal)		N1-C11-C12-C13	54.3(4)	gauche (synclinal)
	C11-C12-C13-N3	54.6(1)	gauche (synclinal)		C11-C12-C13-N3	50.4(4)	gauche (synclinal)
	C12-C13-N3-C14	86.8(5)	anticlinal		C12-C13-N3-C14	91.2(4)	anticlinal
	C13-N3-C14-O2	1.1(2)	eclipsado (synperiplanar)		C13-N3-C14-02	-2.4(5)	eclipsado (synperiplanar)

(*)The conformations have been described using the Klyne-Prelog system. (**) CrystEngComm 19, 1076–1088.

Symmetry Codes: $\mathbf{L^1}$, (a) *-x,y,-z+1/2*; **2**, (a) *-x+1,-y,-z+1/2*

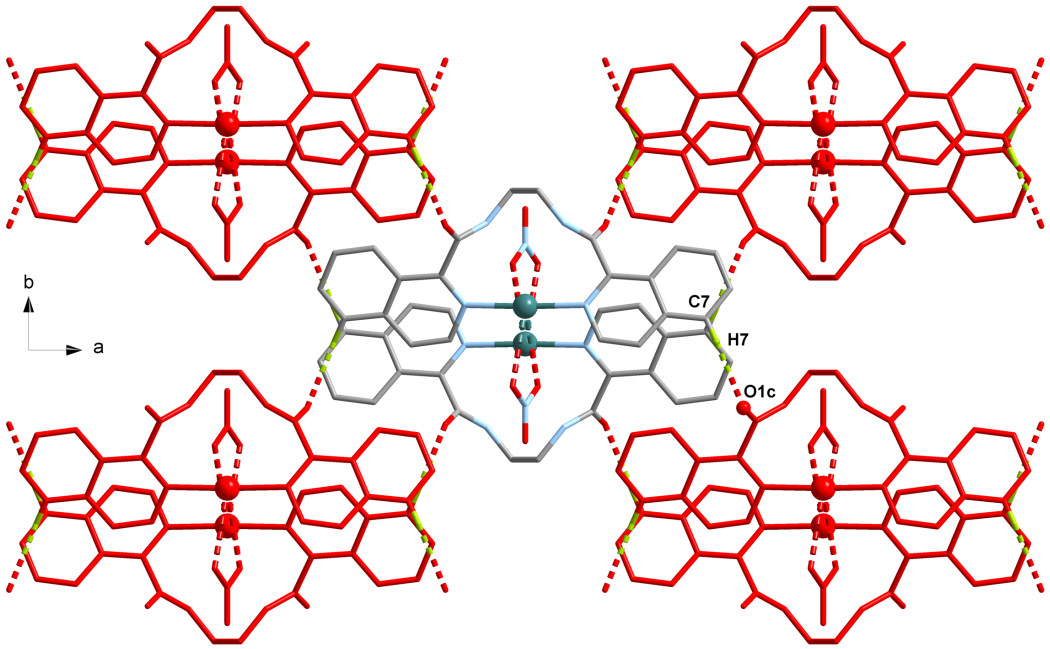

Figure S1. Crystal packing of compound **2**, each supramolecular chain, running along *c* axis, is connected to other four (red) by C-H···$O_{(amide)}$ interactions.

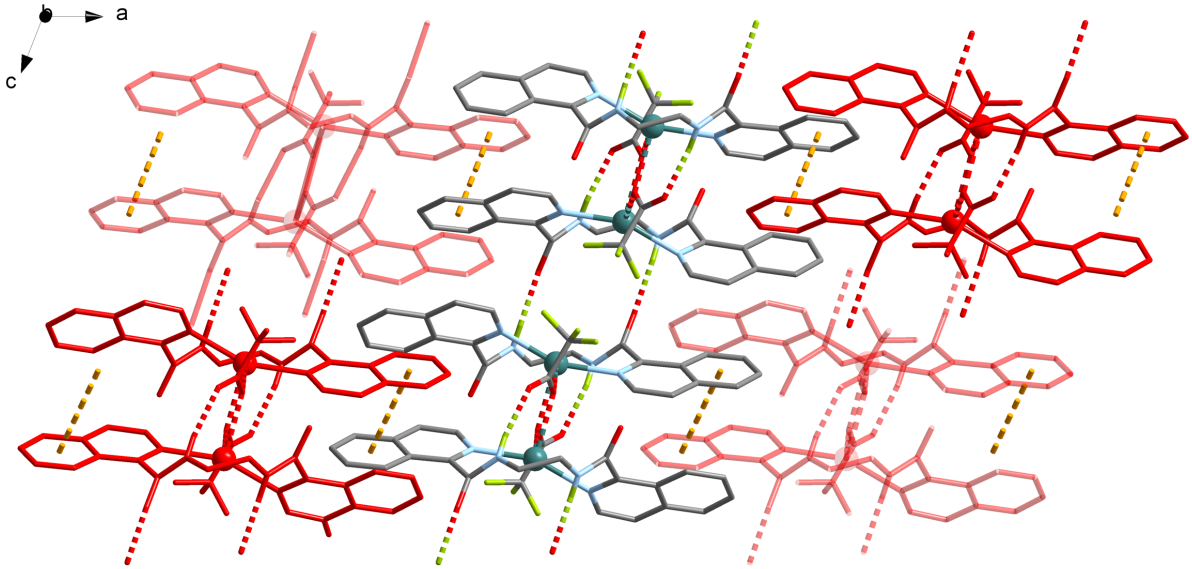

Figure S2. Crystal packing of **3**, the π-π interactions (yellow dashed lines) connect four supramolecular chains (two red in front and two red behind).

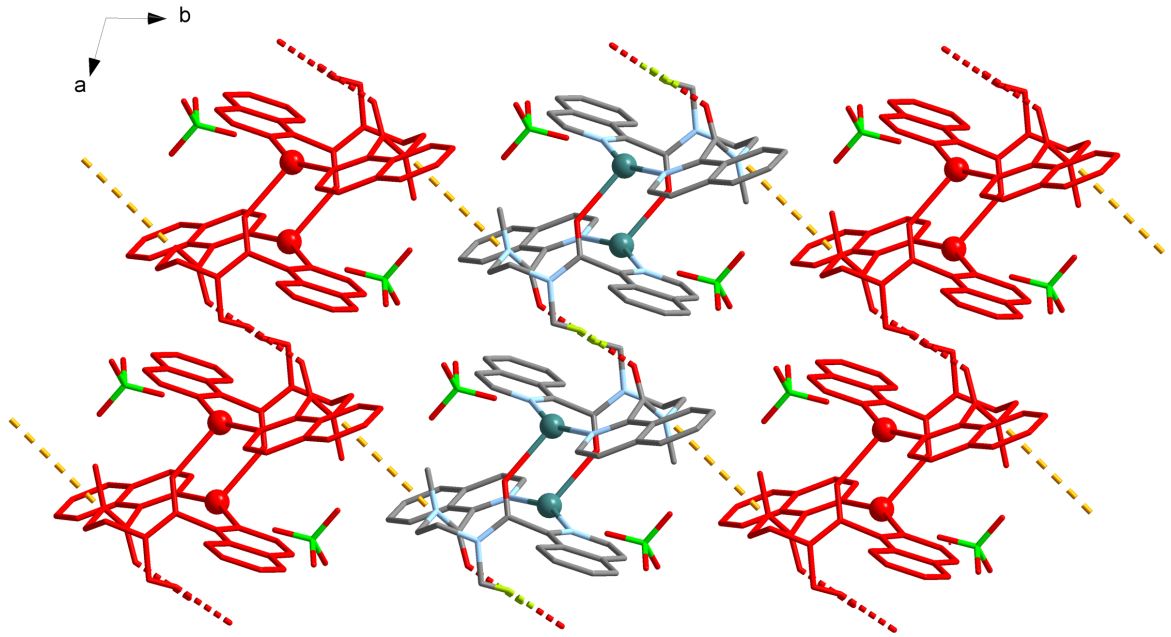

Figure S3. Supramolecular packing of **4**, connection of polymeric chains through π-π interactions (yellow dashed lines) along *ab* plane.

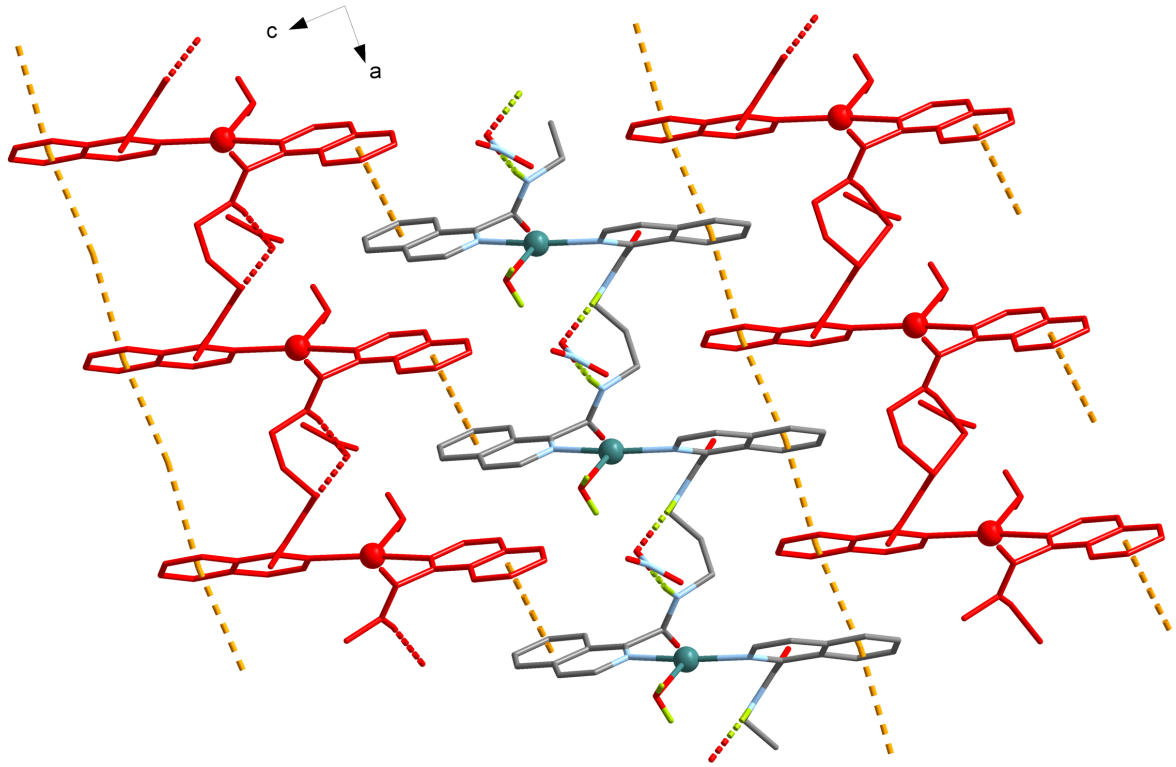

Figure S4. Crystal packing of **8**, connection of polymeric chains through π-π interactions (yellow dashed lines) along *ac* plane.

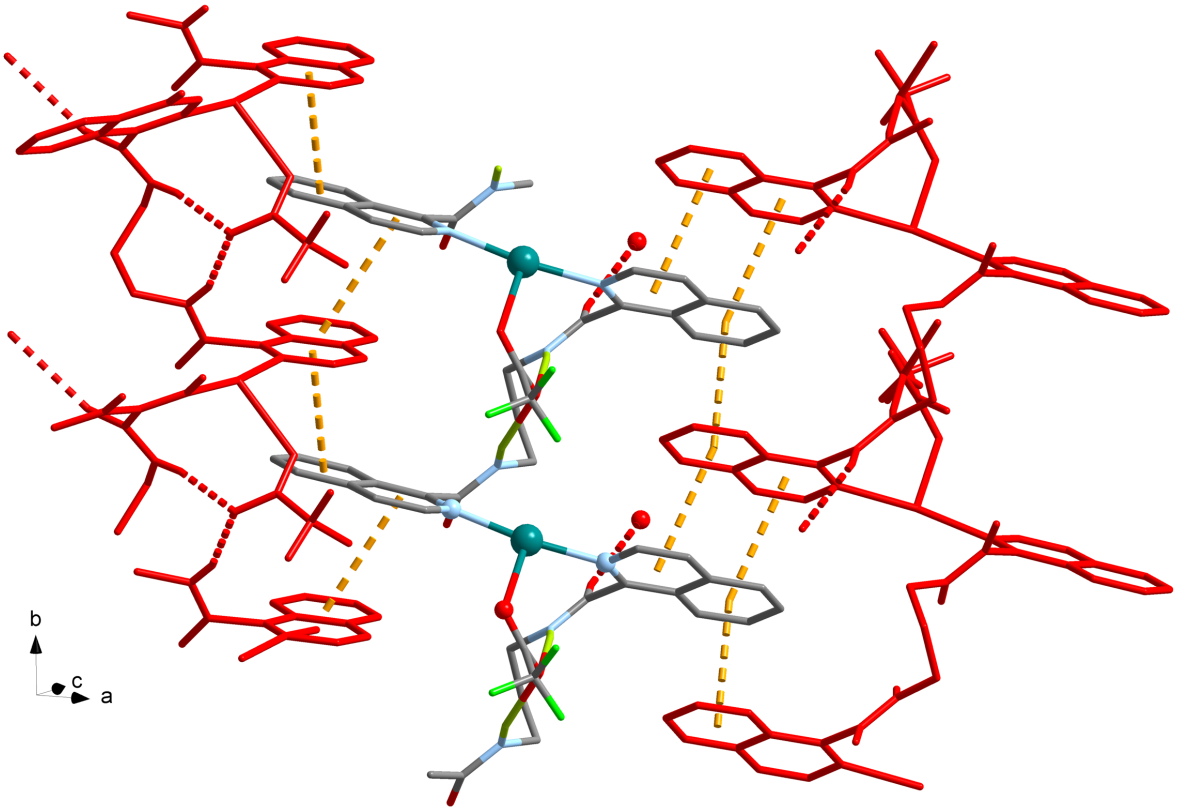

Figure S5. Supramolecular packing of **9**, connection of polymeric chains through π-π interactions (yellow dashed lines).

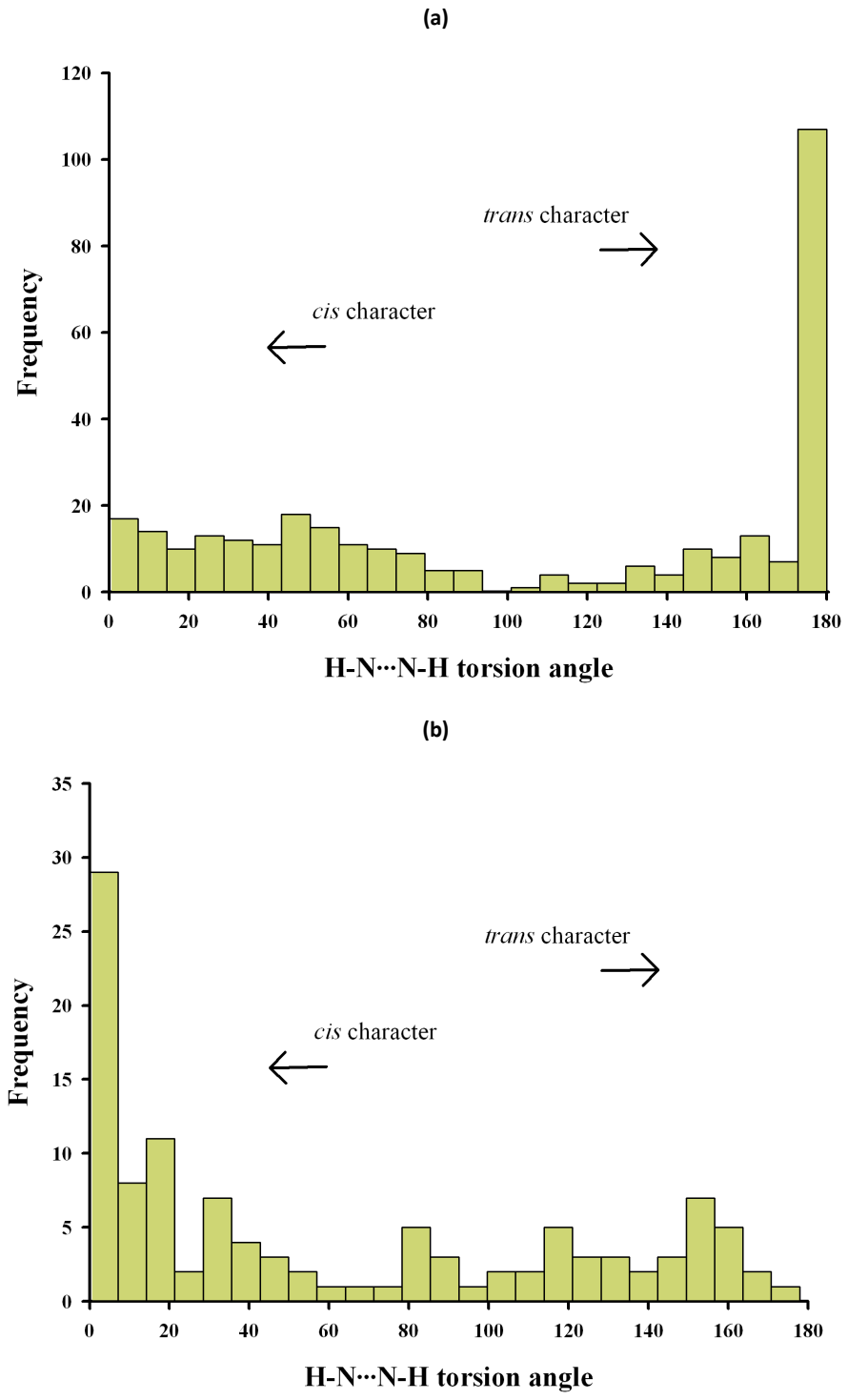

Figure S6. Histogram of the frequency of cis/trans orientation of the amide group in (**a**) C2 or (**b**) C3 chain lengths.