Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

SUPPLEMENTARY DATA

Transformations of the natural cytokinin N6-isopentenyladenine in aqueous acidic media: structural aspects

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Table S1. Hydrogen-bond parameters in **1** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
N6–H6···Cl1	0.86(4)	2.372(11)	3.206(4)	163.5(2)
N9–H9···O1	0.86(4)	1.888(3)	2.726(5)	164.6(3)
O1–H1V···Cl2^{i}	0.88(5)	2.30(5)	3.178(3)	175.6(4)
N1–H1···Cl2^{ii}	0.86(4)	2.317(11)	3.127(3)	157.0(2)

Symmetry codes: (i) x, 0.5 – y, –0.5 + z; (ii) 1 – x, –0.5 + y, 0.5 – z

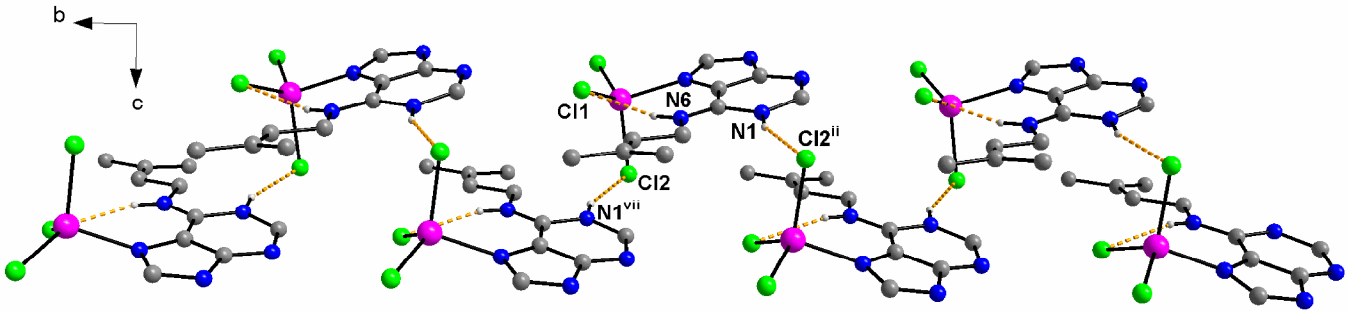

Fig. S1. A part of the crystal structure of complex [Zn(HL1)Cl_3]·H_2O (**1**). A view along the *a* axis showing the formation of N–H···Cl hydrogen bonds arranging the molecules into two-layered infinite chains. The hydrogen atoms not involved in the hydrogen bonds, the water molecules of crystallization and the disordered atoms with the occupancy factor 0.181(8) have been omitted for clarity. Symmetry codes: (i) x, 0.5 – y, –0.5 + z; (ii) 1 – x, –0.5 + y, 0.5 – z.

Table S2. Hydrogen-bond parameters in **2** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
N6A–H6A···Cl7	0.77(3)	2.41(3)	3.166(3)	170.6(4)
N9–H9···Cl2^{i}	0.86(3)	2.327(6)	3.157(3)	162.4(2)
N9A–H9A1···N3A^{ii}	0.86(3)	2.031(2)	2.865(3)	163.1(2)

Symmetry codes: (i) $-1+x, y, z$; (ii) $1-x, -y, 1-z$

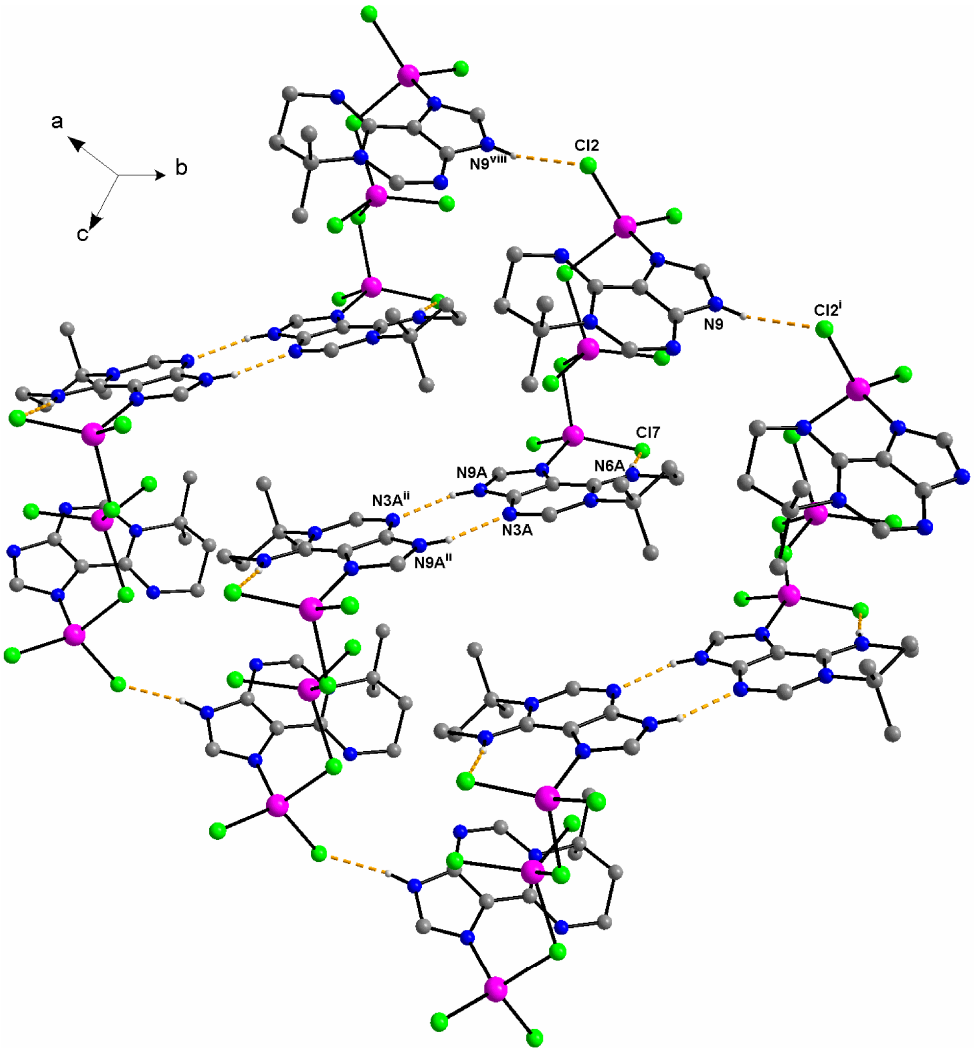

Fig. S2. A part of the crystal structure of complex $[Zn_3(HL2)_2Cl_8]$ (**2**) showing the formation of N–H···N and N–H···Cl hydrogen bonds. The N–H···N hydrogen bonds arrange the molecules into centrosymmetric dimers. The hydrogen atoms not involved in hydrogen bonds and the disordered

atoms with the occupancy factor 0.216(3) have been omitted for clarity. Symmetry codes: (i) –1 + *x*, *y*, *z*; (ii) 1 – *x*, –*y*, 1 – *z*; (viii) 1 + *x*, *y*, *z*.

Table S3. Hydrogen-bond parameters in **3** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
N8–H8···Cl2	0.88(11)	2.286(3)	3.135(12)	161.93(8)
N1–H1···O1	0.88(13)	1.869(11)	2.674(2)	151.11(9)
O1–H1W···O2	0.868(14)	1.934(14)	2.780(2)	164.2(14)
O1–H1V···Cl1	0.88(2)	2.31(2)	3.173(13)	166.8(2)
O2–H2V···Cl1^{i}	0.88(2)	2.274(2)	3.139(13)	169.7(2)
O2–H2W···Cl2^{i}	0.89(2)	2.29(2)	3.177(13)	175.7(2)
N6–H6A···Cl2^{ii}	0.85(2)	2.347(2)	3.176(2)	163.6(2)
N3–H3···Cl1^{iii}	0.88(12)	2.577(4)	3.319(13)	130.53(8)

Symmetry codes: (i) 1 + *x*, *y*, *z*; (ii) 1 – *x*, 1 – *y*, –*z*; (iii) 0.5 + *x*, 1.5 – *y*, –0.5 + *z*

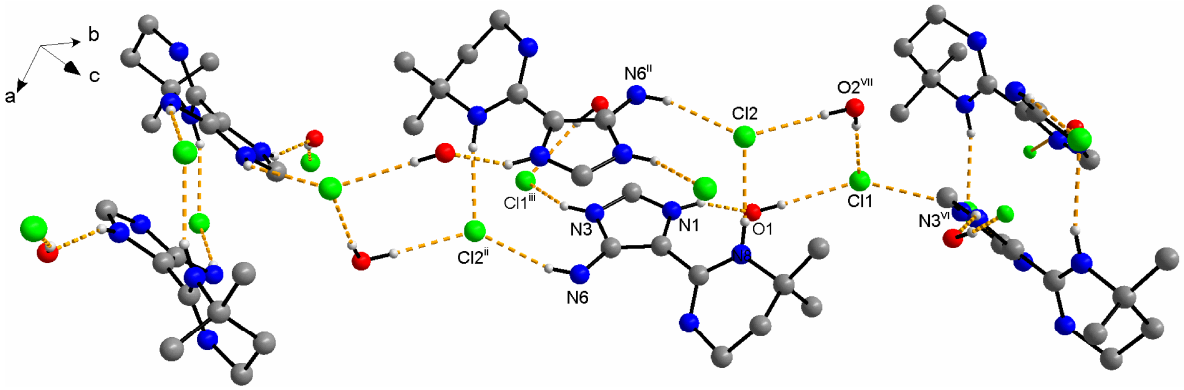

Fig. S3. A part of the crystal structure of $(H_2L3)Cl_2{\cdot}2H_2O$ (**3**) showing the formation of N–H···N and N–H···Cl hydrogen bonds. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity. Symmetry codes: (ii) 1 – *x*, 1 – *y*, –*z*; (iii) 0.5 + *x*, 1.5 – *y*, –0.5 + *z*; (vi) –0.5 + *x*, 1.5 – *y*, 0.5–*z*; (vii) –1 + *x*, *y*, *z*.

Table S4. Hydrogen-bond parameters in **4** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
N9–H9···Cl4	0.88(2)	2.358(7)	3.154(2)	150.5(2)
N11–H11···Cl3^{i}	0.88(2)	2.291(7)	3.134(2)	160.4(2)
N6–H6···Cl3^{ii}	0.88(2)	2.408(7)	3.247(2)	159.6(2)

Symmetry codes: (i) $-x$, $1-y$, $1-z$; (ii) $-x$, $2-y$, $1-z$

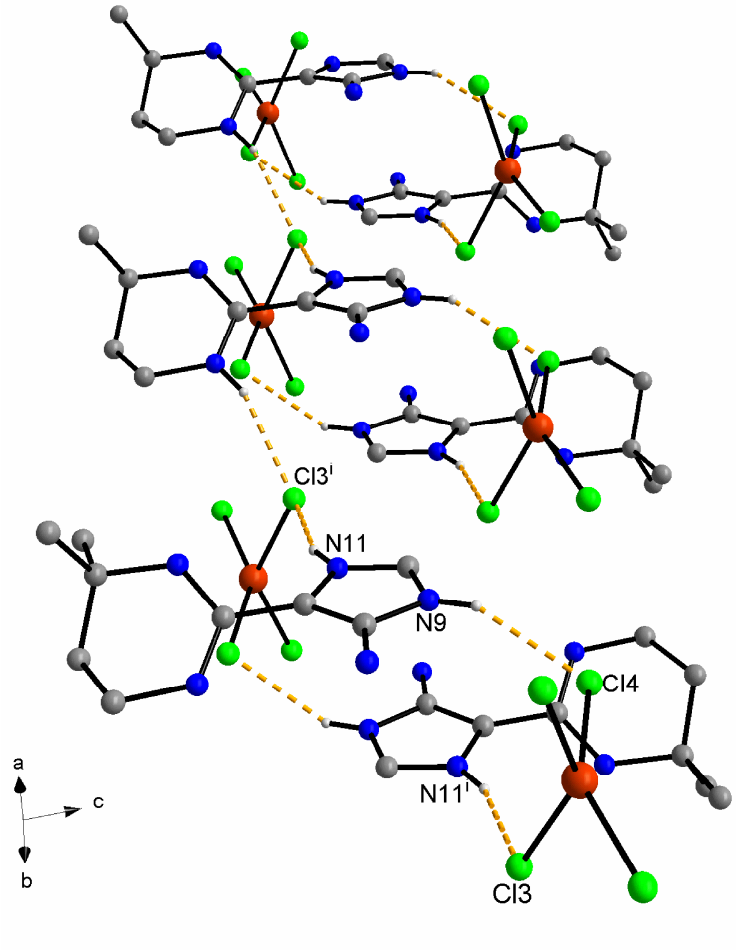

Fig. S4. A part of the crystal structure of $(H_2L3)[CuCl_4]$ (**4**) showing the formation of N–H···Cl hydrogen bonds. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity. Symmetry code: (i) $-x$, $1-y$, $1-z$.

Table S5. Hydrogen-bond parameters in **5** (Å, °)

D–H···A	**D–H**	**H···A**	**D···A**	**D–H···A**
N3–H3···Cl9	0.88(3)	2.390(6)	3.226(3)	158.6(2)
N3′–H3′···Cl4	0.88(3)	2.420(8)	3.207(3)	149.1(2)
N6–H6A···Cl3^{i}	0.87(4)	2.409(4)	3.239(3)	160.7(3)
N1–H1···Cl7^{ii}	0.88(3)	2.340(9)	3.185(3)	161.1(2)
N12′–H12′···Cl5^{ii}	0.88(2)	2.454(7)	3.239(2)	148.7(2)
N1′–H1′···Cl8^{ii}	0.88(3)	2.275(9)	3.148(3)	171.9(2)
N8′–H8′···Cl5^{iii}	0.88(3)	2.388(7)	3.247(3)	165.7(2)
N8–H8···Cl9^{iv}	0.88(3)	2.418(7)	3.235(3)	154.6(2)

Symmetry codes: (i) x, $1 + y$, z; (ii) $-x$, $1 - y$, $1 - z$; (iii) $1 - x$, $1 - y$, $1 - z$; (iv) $1 - x$, $2 - y$, $1 - z$

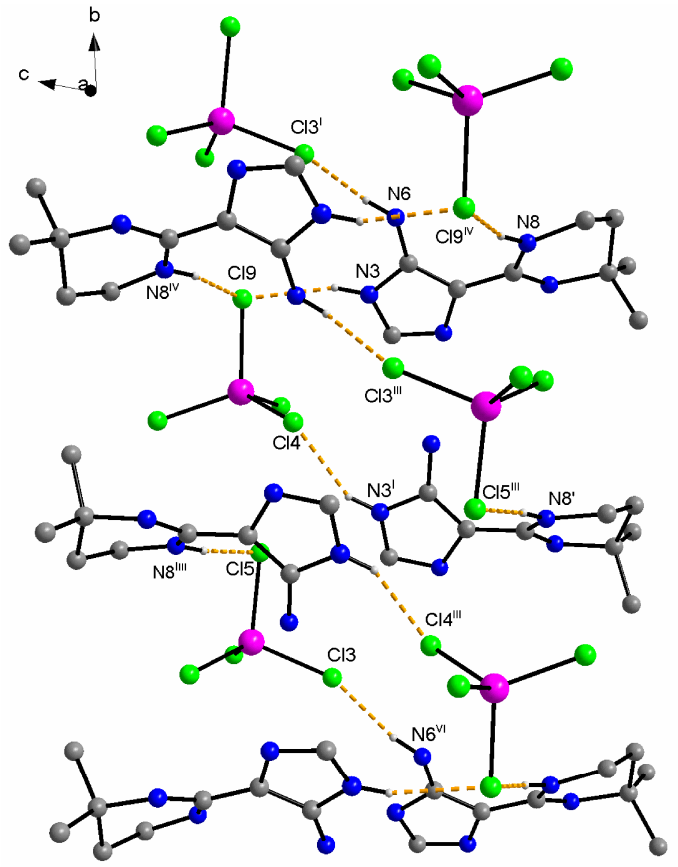

Fig. S5. A part of the crystal structure of $(H_2L3)[ZnCl_4]$ (**5**) showing the N–H···Cl hydrogen bond formation. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity. Symmetry codes: (i) x, $1 + y$, z; (iii) $1 - x$, $1 - y$, $1 - z$; (iv) $1 - x$, $2 - y$, $1 - z$; (i) x, $-1 + y$, z.