Supplementary information

For the manuscript "Coordination Polymers and molecular complexes of Group 13 Metal Halides with Bis-pyridylethane: comparison with rigid N-containing ligands" by Nikita Y. Gugin,[a] Alexander V. Virovets,[b] Eugenia Peresypkina,[c] Elena I. Davydova,[a] and Alexey Y. Timoshkin [a]

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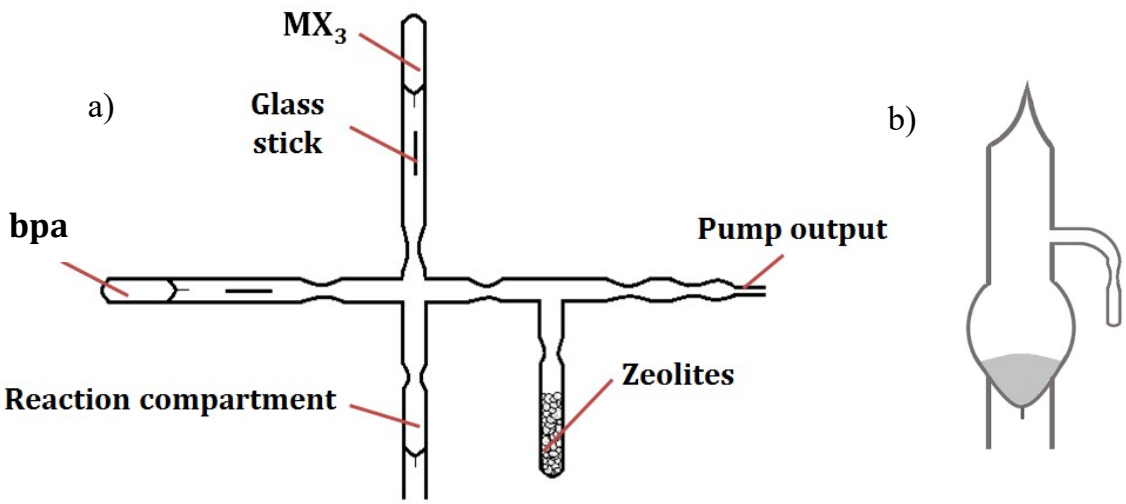


Fig. S1 a) A schematic view of the system for synthesis; b) A sealed glass ampoule with the reagent mixture and a compartment for the excess reagent (optional).

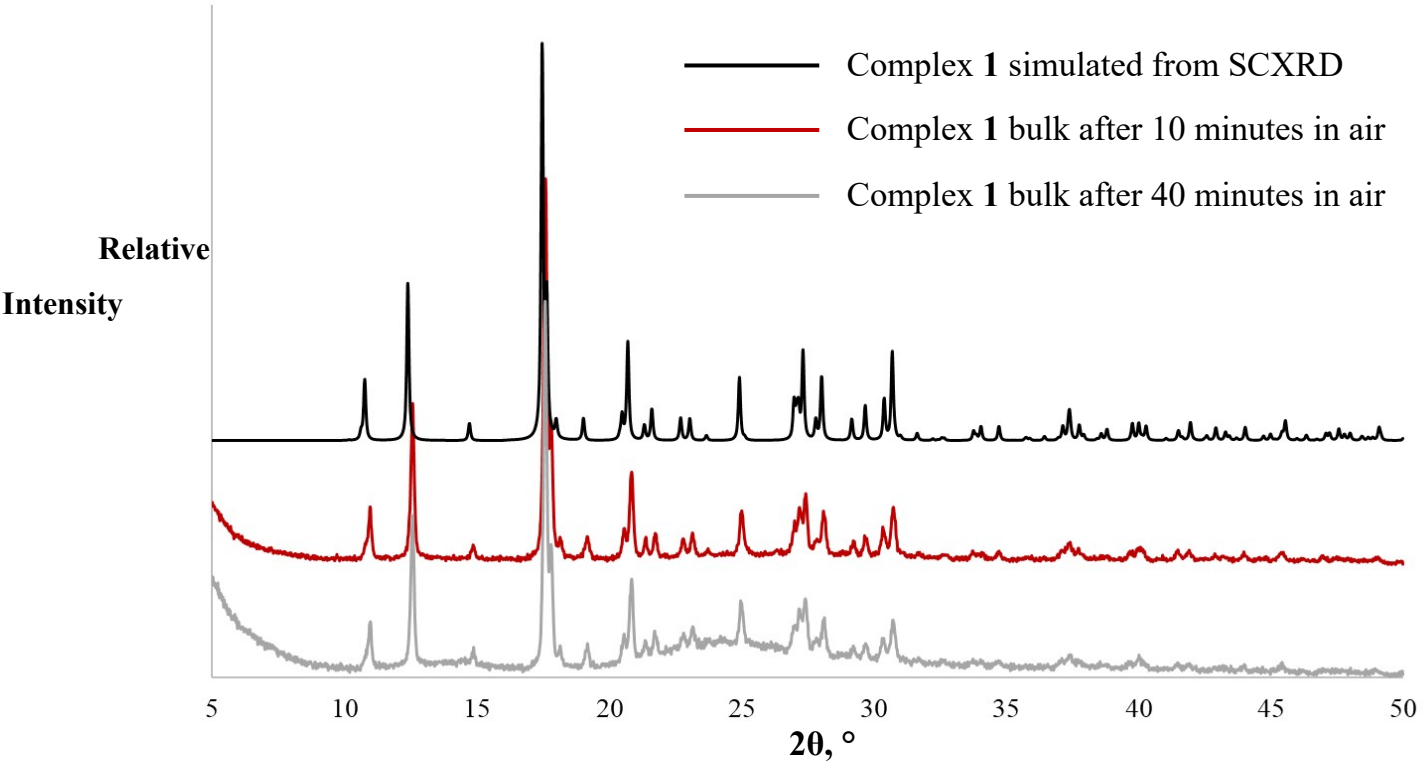


Fig. S2 Comparison of the simulated (black) and experimental diffraction patterns of **1** after 10 (red) and 40 minutes (grey) in air (Cu-Kα1 = 154.1 pm).

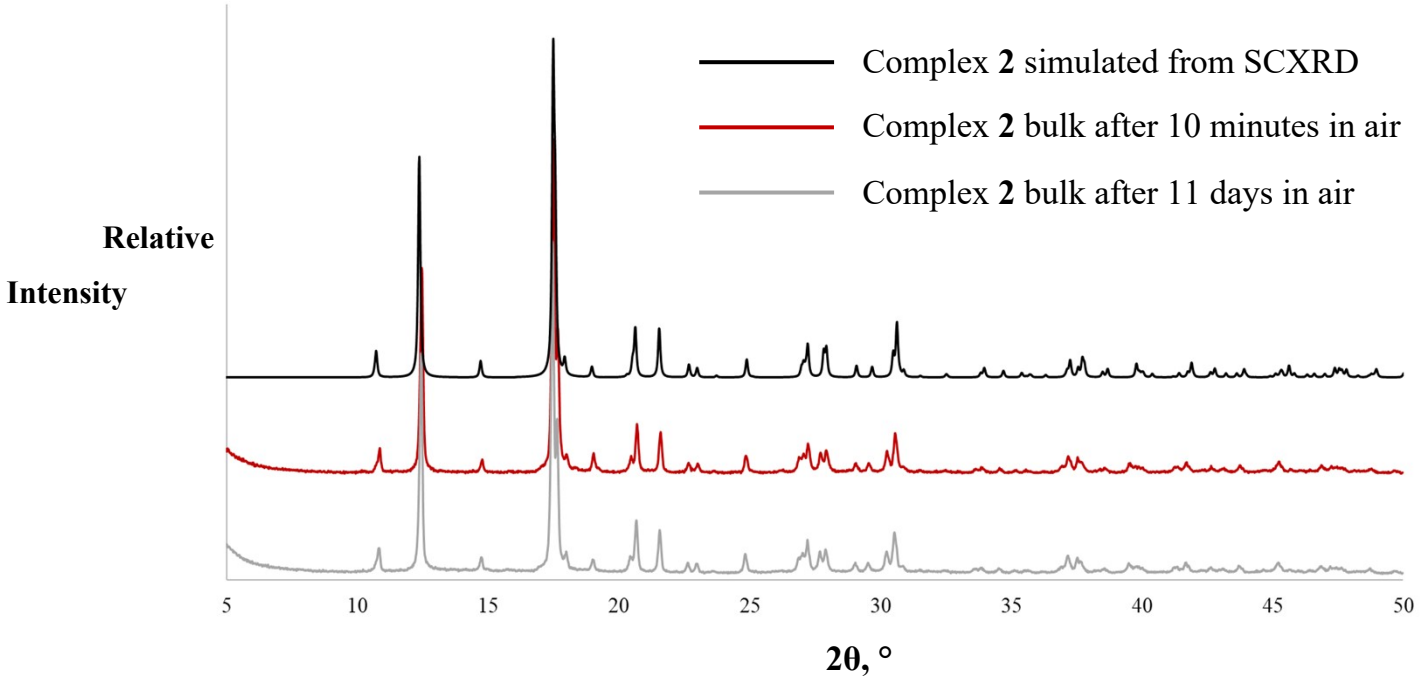


Fig. S3 Comparison of the simulated (black) and experimental diffraction patterns of **2** after 10 minutes (red) and 11 days (grey) in air (Cu-Kα1 = 154.1 pm).

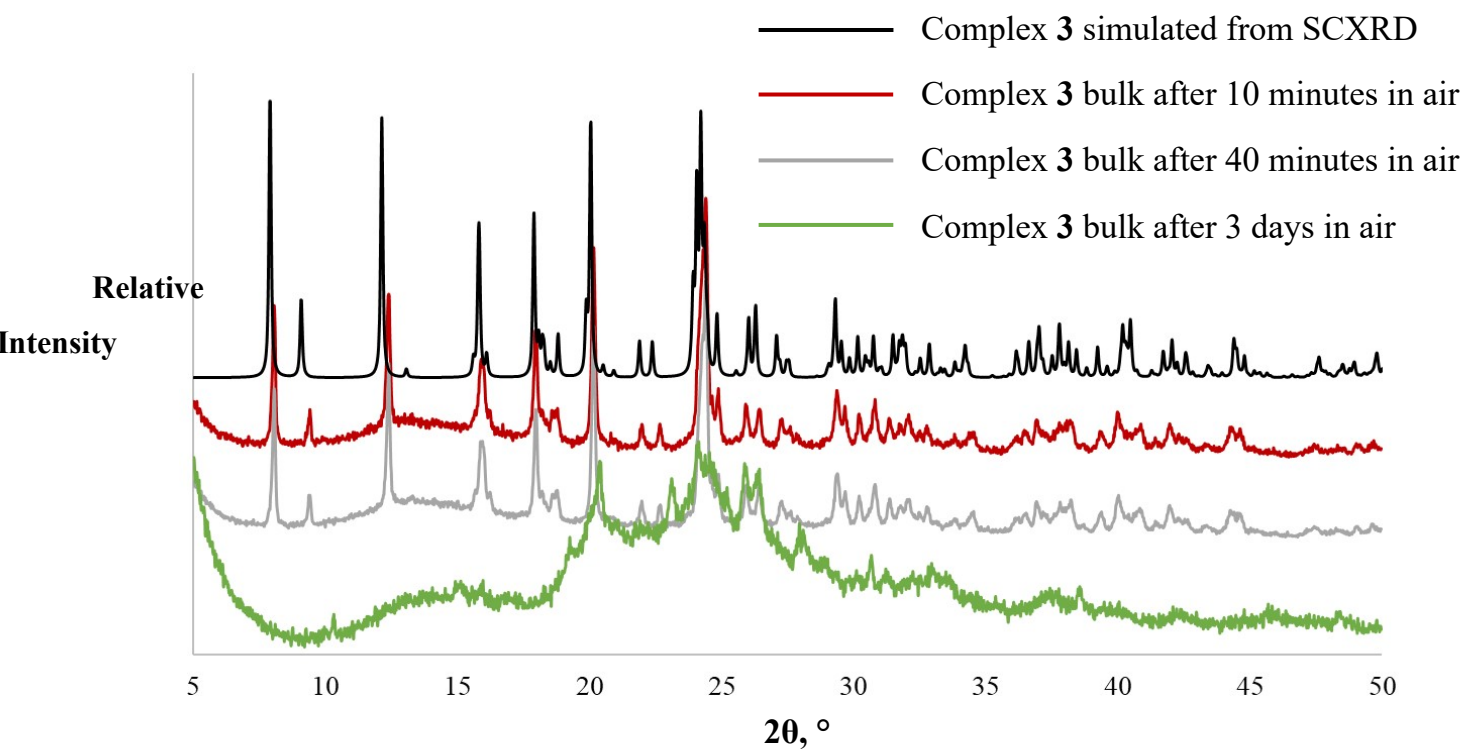


Fig. S4 Comparison of the simulated (black) and experimental diffraction patterns of **3** after 10 minutes (red), 40 minutes (grey) and 3 days (green) in air (Cu-Kα1 = 154.1 pm).

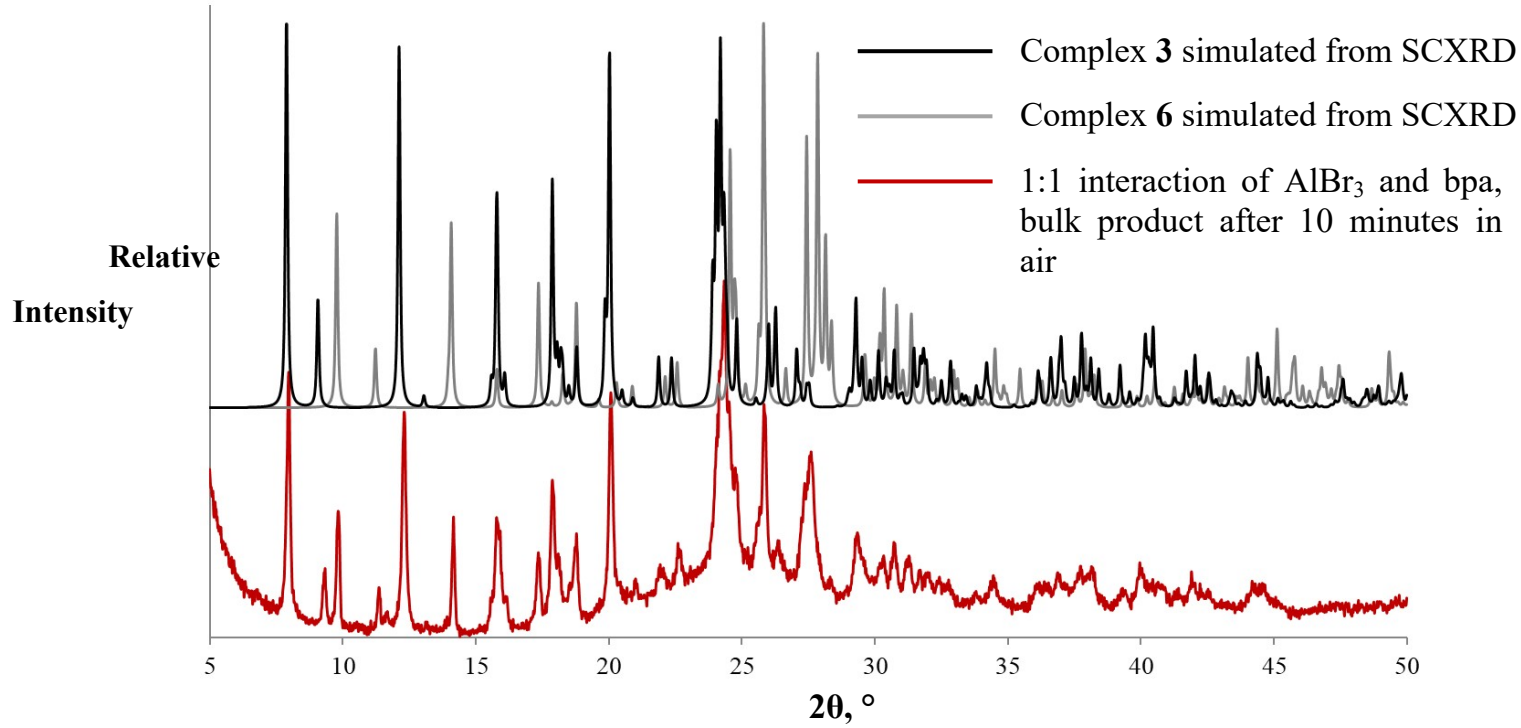


Fig. S5 Comparison of the experimental diffraction patterns of the bulk product of the 1:1 interaction of $AlBr_3$ and bpa after 10 minutes in air (red, bottom) and simulated diffraction patterns of **3** (black, top) and **6** (grey, top) (Cu-Kα1 = 154.1 pm).

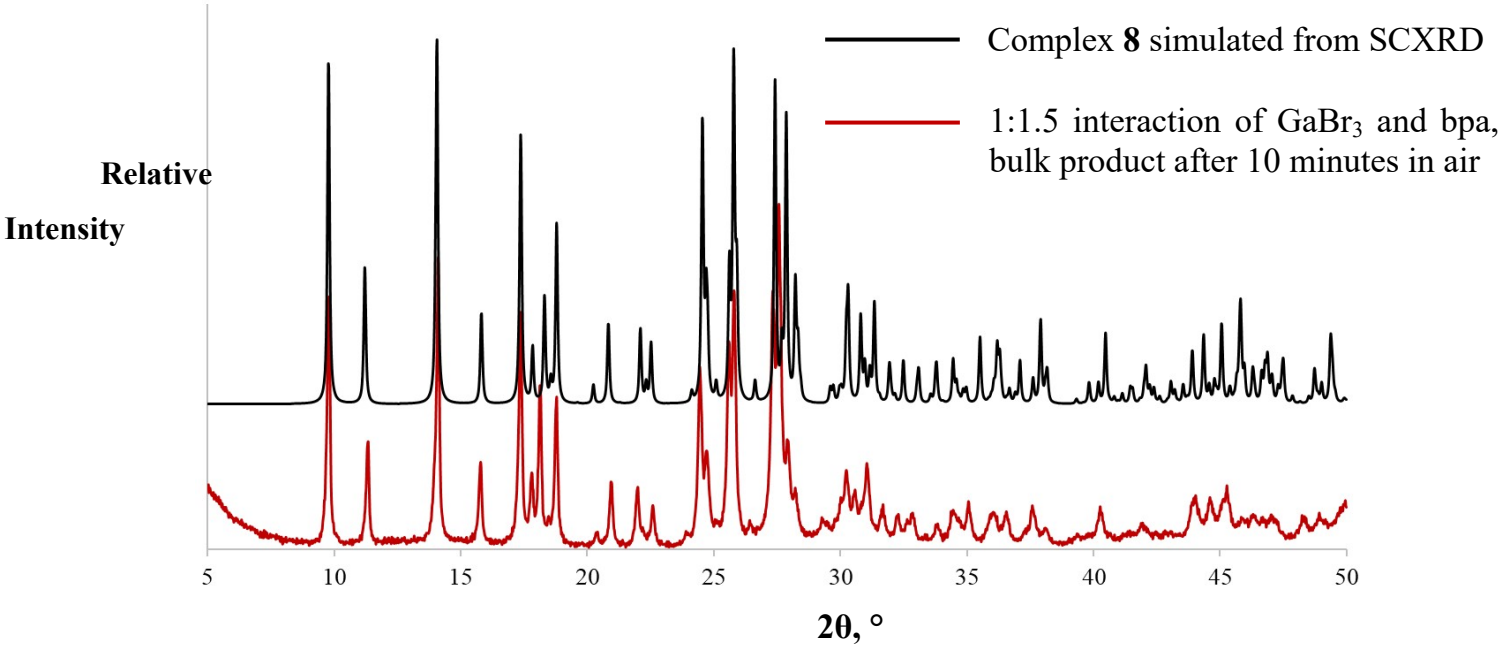


Fig. S6 Comparison of the experimental diffraction patterns of the bulk product of the 1:1.5 interaction of $GaBr_3$ and bpa after 10 minutes in air (red, bottom) and simulated diffraction patterns of **8** (black, top) (Cu-Kα1 = 154.1 pm).

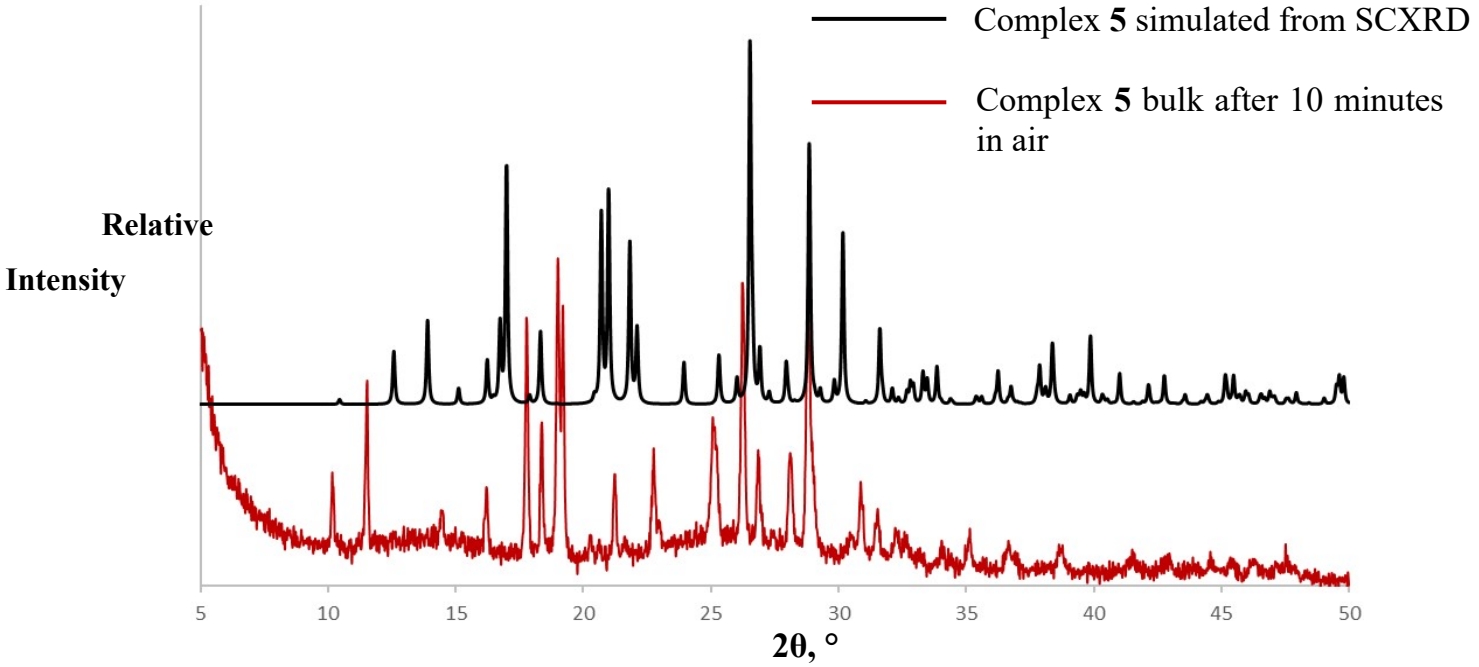


Fig. S7 Comparison of the simulated (black, top) and experimental (red, bottom) diffraction pattern of **5** after 10 minutes in air (Cu-Kα1 = 154.1 pm).

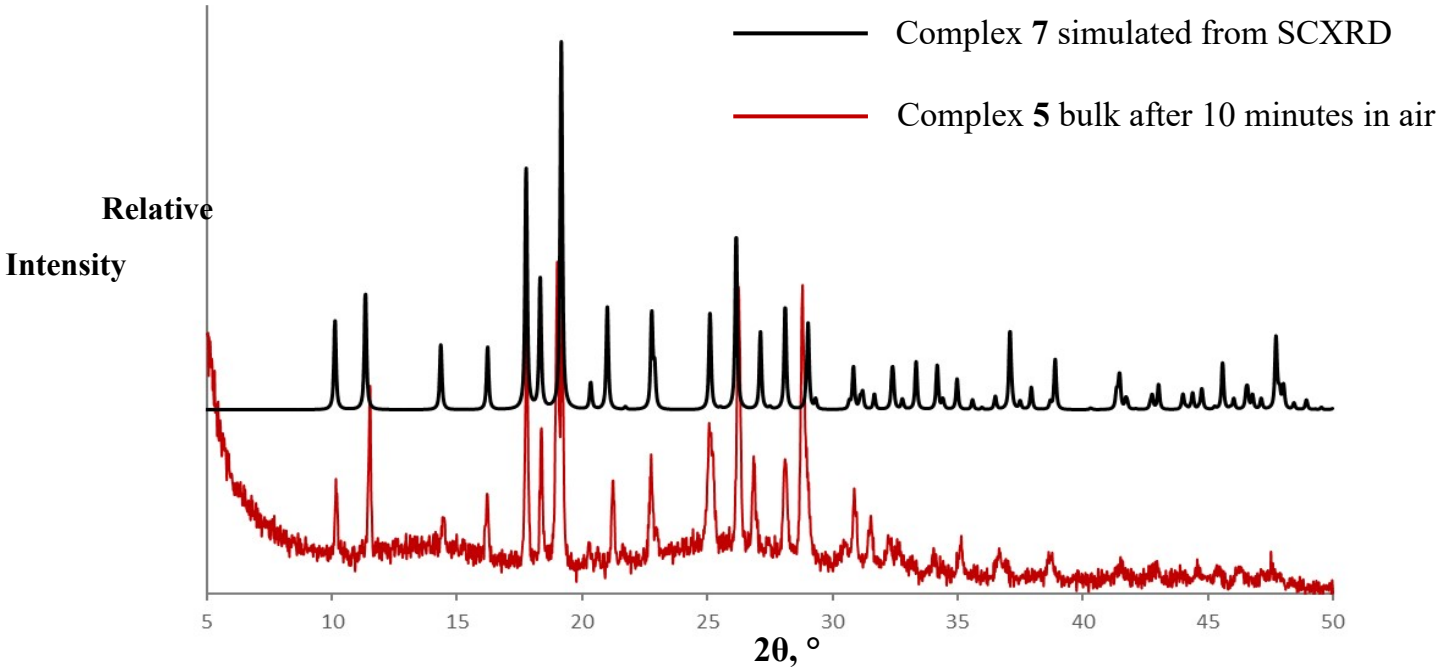


Fig. S8 Comparison of the simulated diffraction pattern of **7** (black, top) and of the experimental diffraction pattern of **5** (red, bottom) after 10 minutes in air (Cu-Kα1 = 154.1 pm).

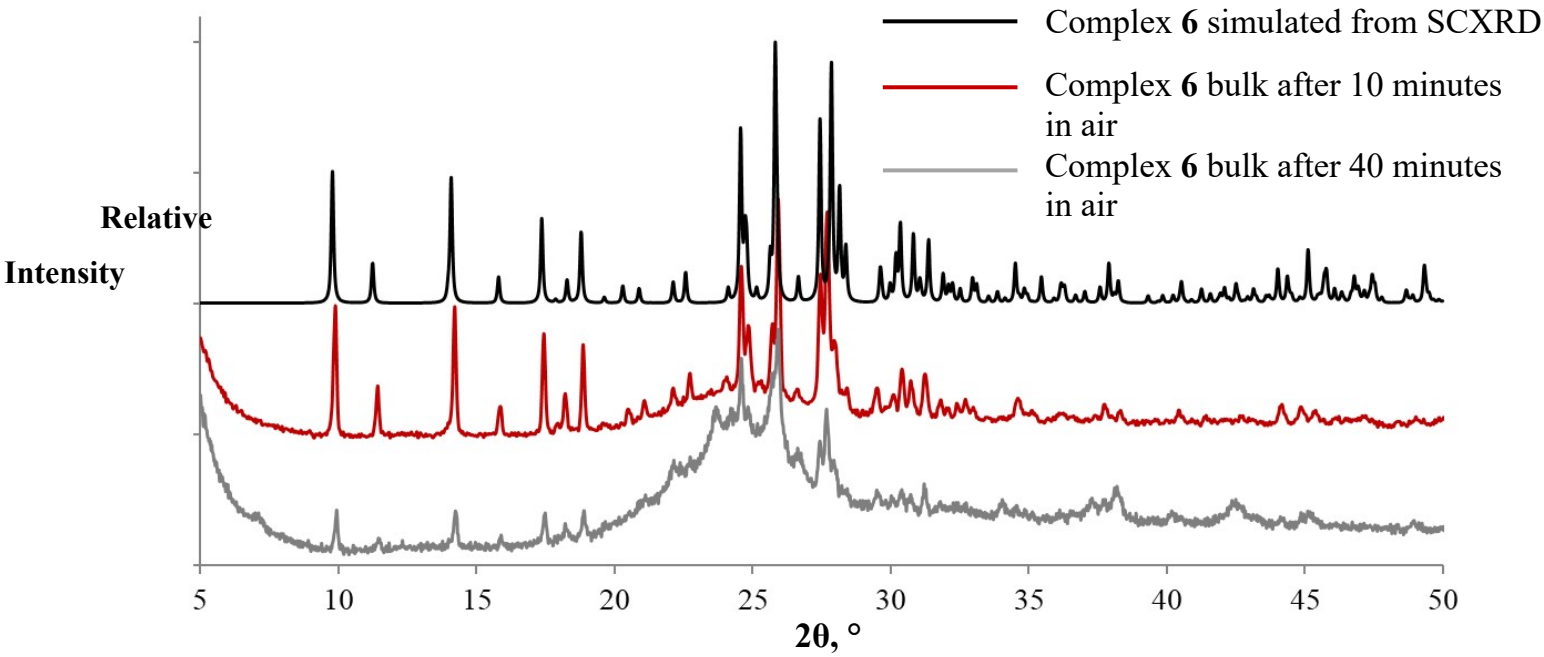


Fig. S9 Comparison of the simulated (black) and experimental diffraction patterns of **6** after 10 (red) and 40 minutes (grey) in air (Cu-Kα1 = 154.1 pm).

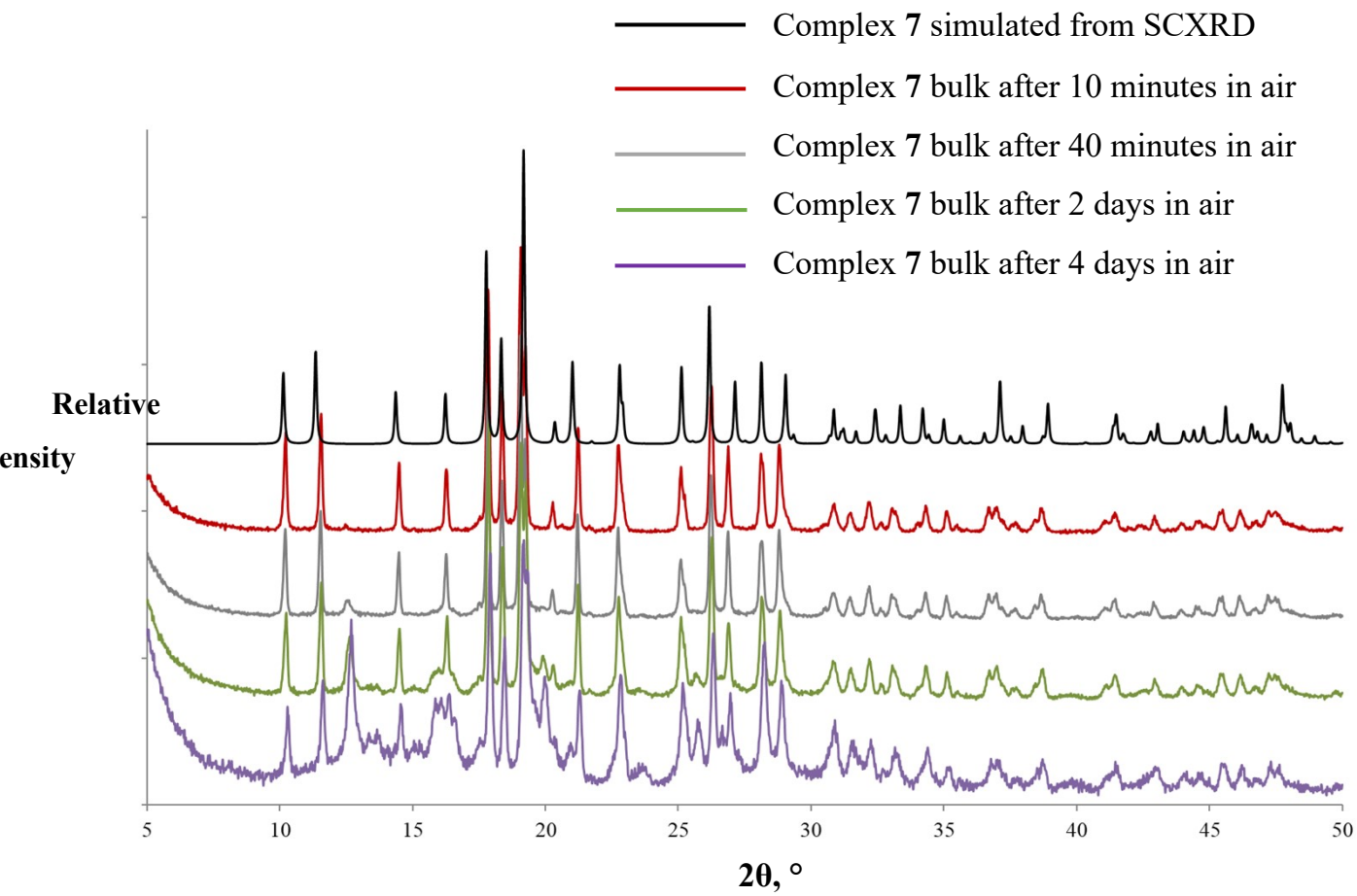


Fig. S10 Comparison of the simulated (black) and experimental diffraction patterns of **7** after 10 minutes (red), 40 minutes (grey), 2 days (green) and 4 days (purple) in air (Cu-Kα1 = 154.1 pm).

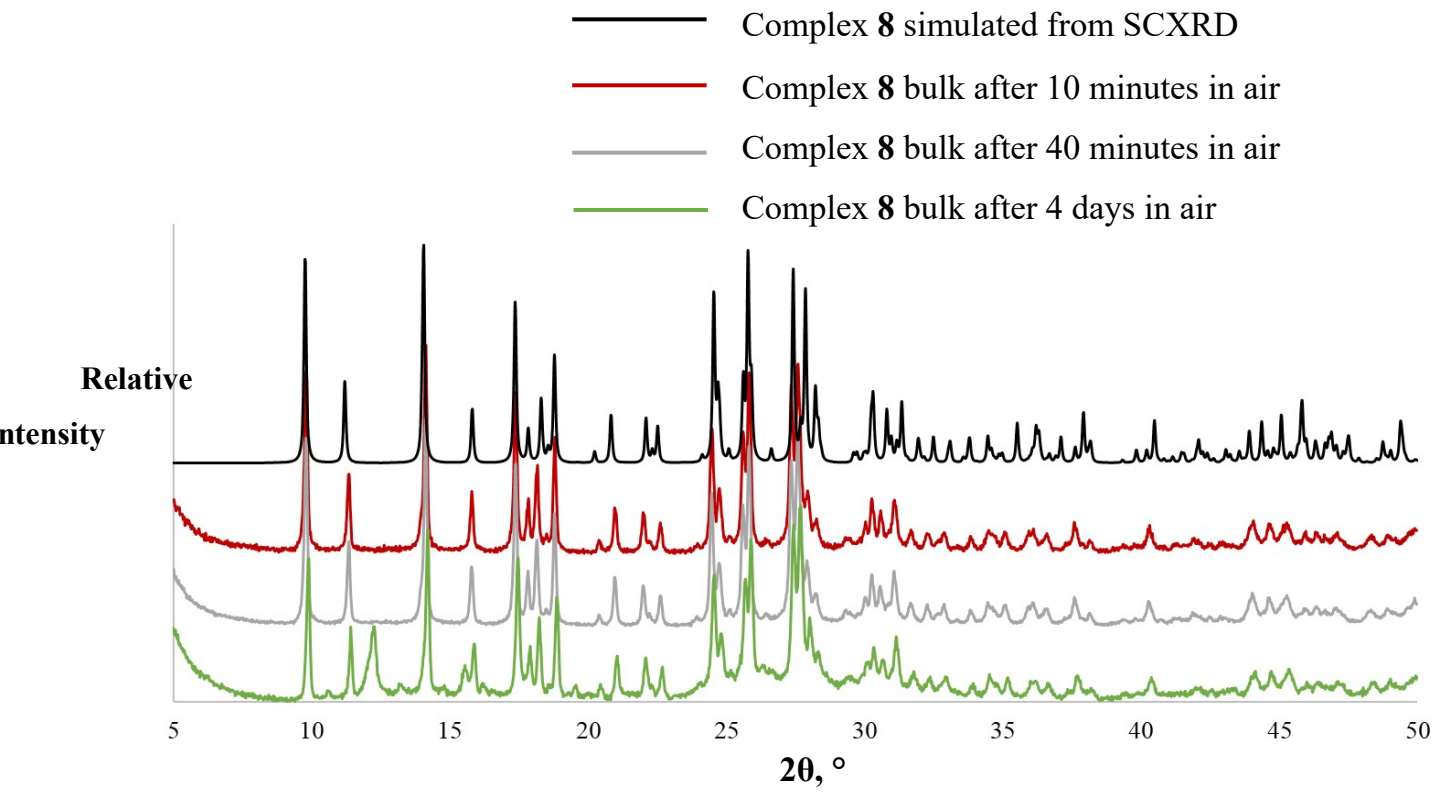


Fig. S11 Comparison of the simulated (black) and experimental diffraction patterns of **8** after 10 minutes (red), 40 minutes (grey) and 4 days (green) in air (Cu-Kα1 = 154.1 pm).

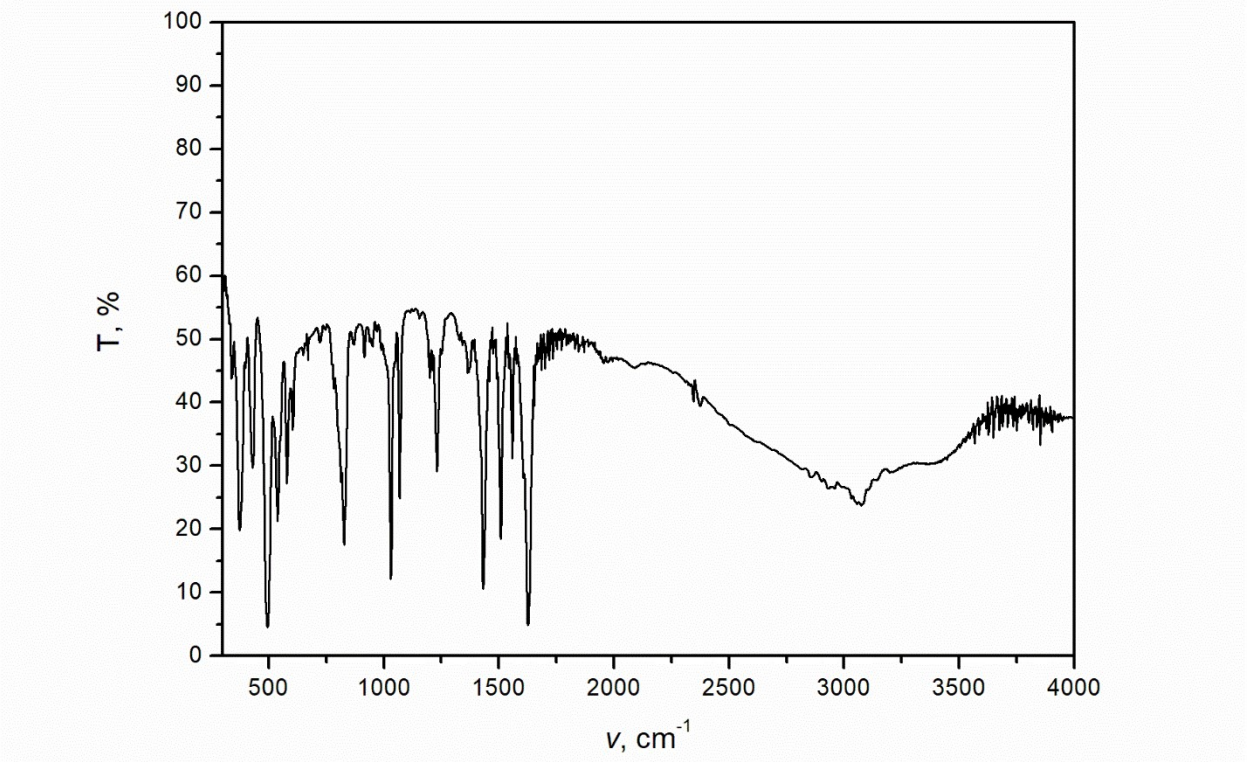


Fig. S12 IR spectrum of **1**.

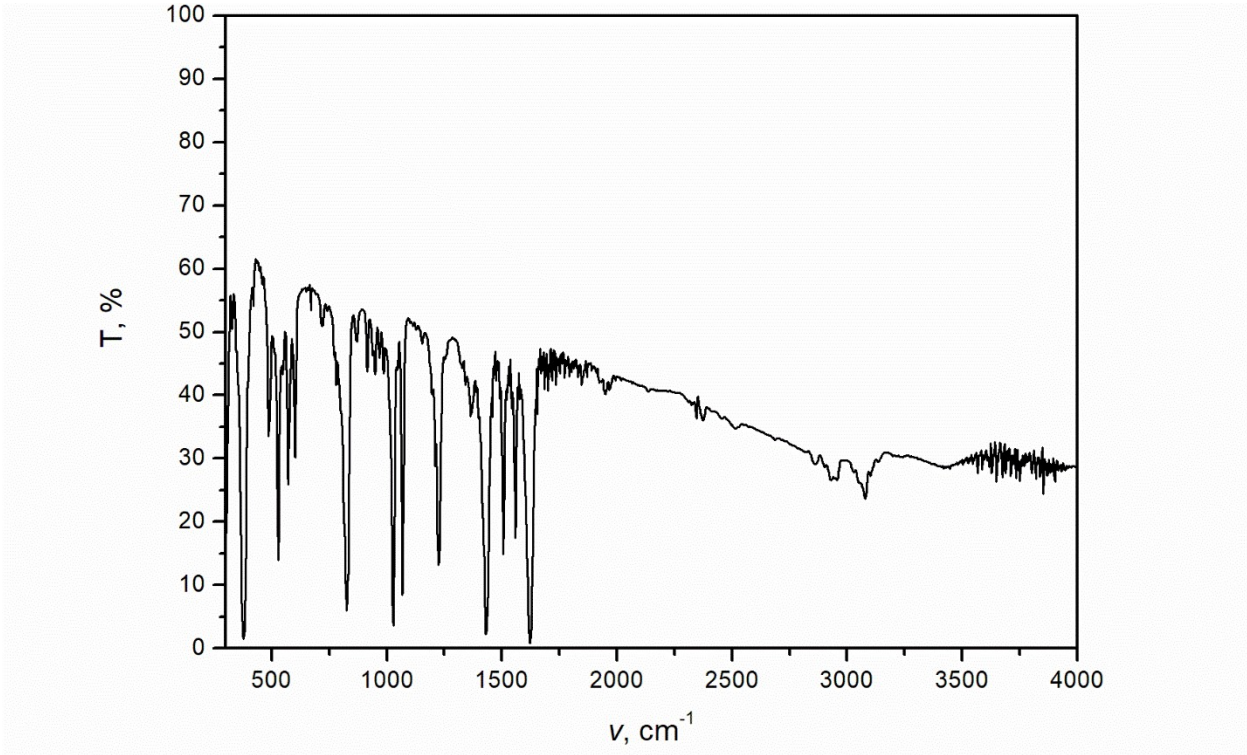


Fig. S13 IR spectrum of **2**.

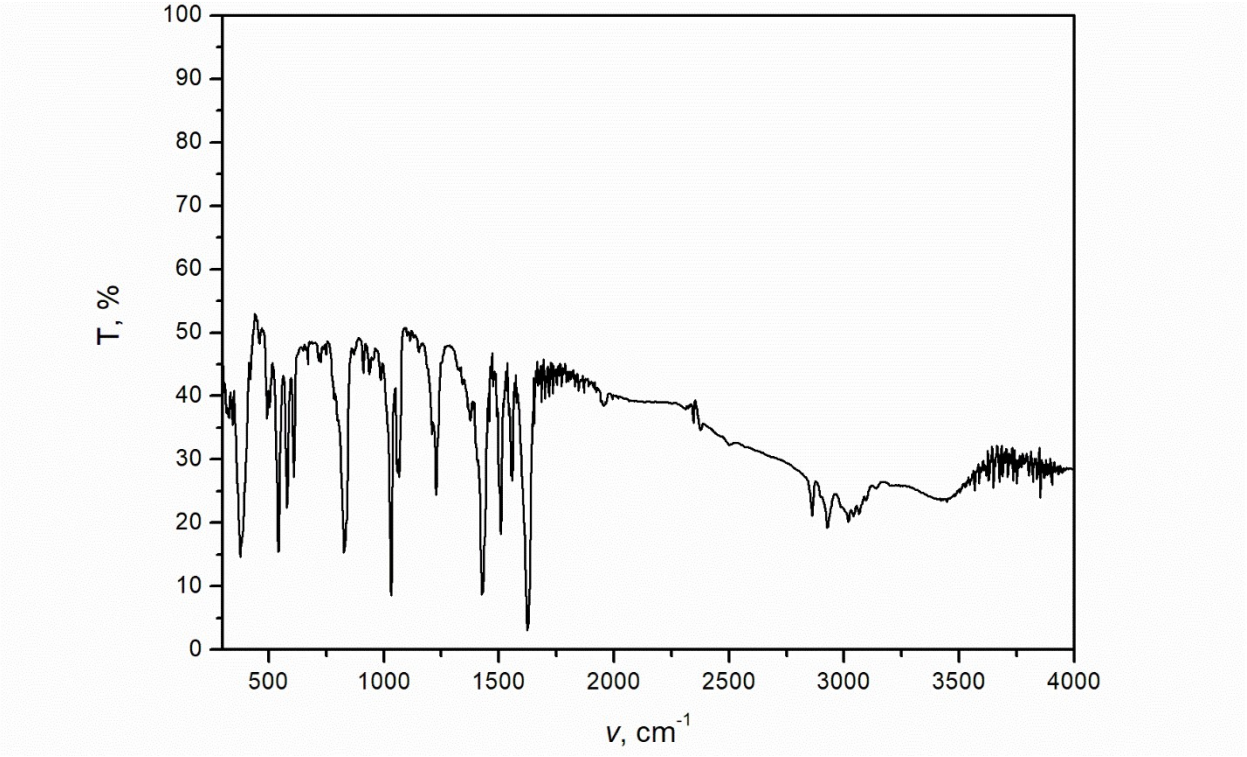


Fig. S14 IR spectrum of **3**.

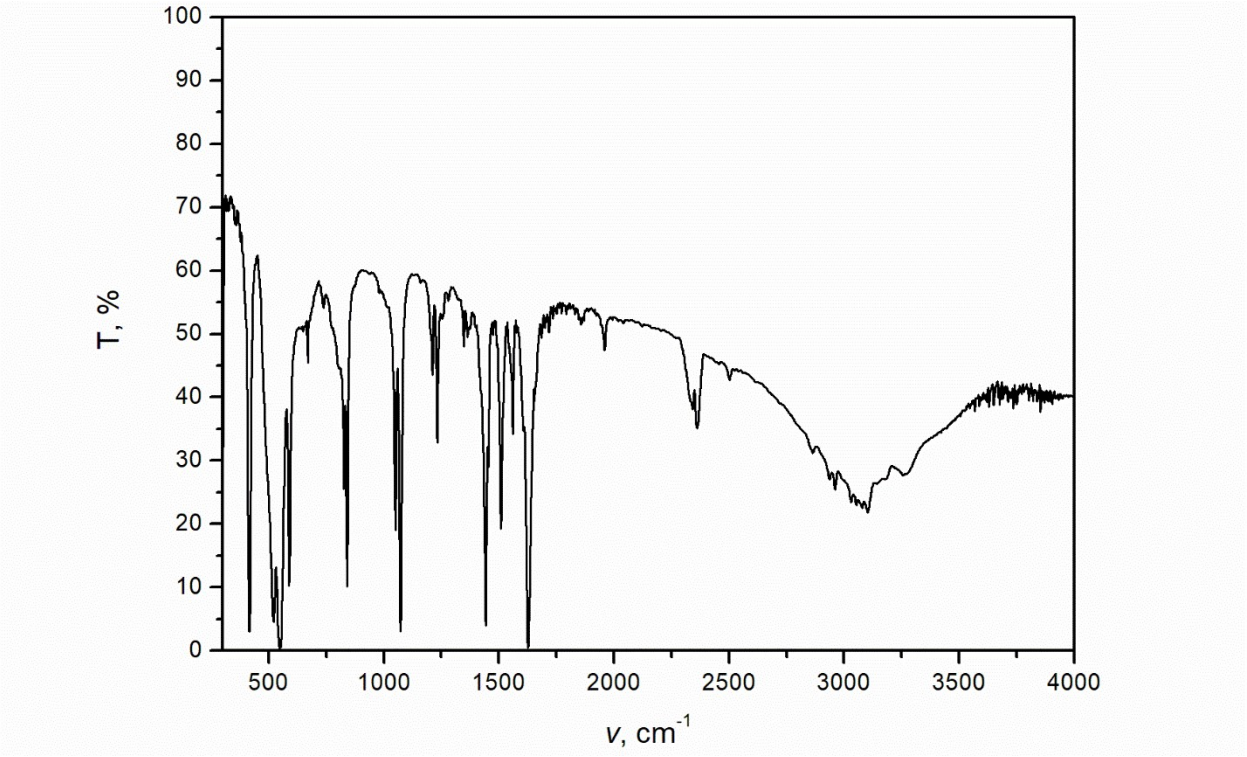


Fig. S15 IR spectrum of **5**.

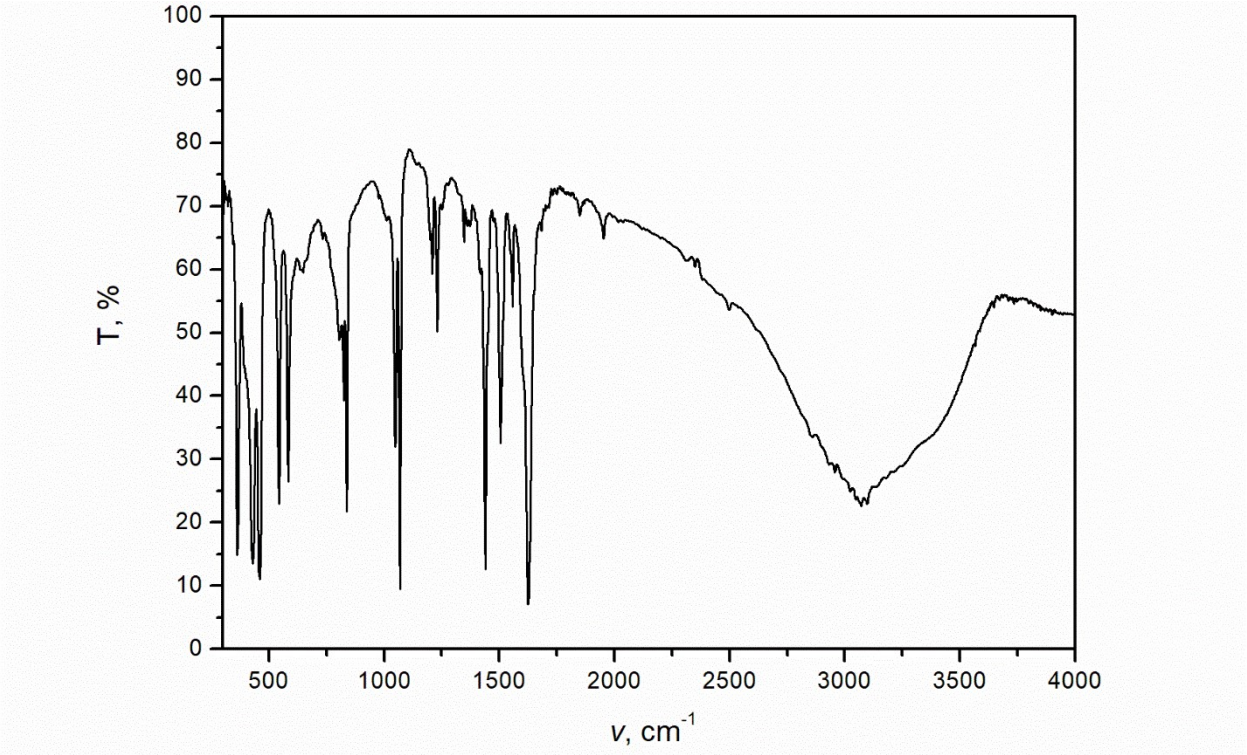


Fig. S16 IR spectrum of **6**.

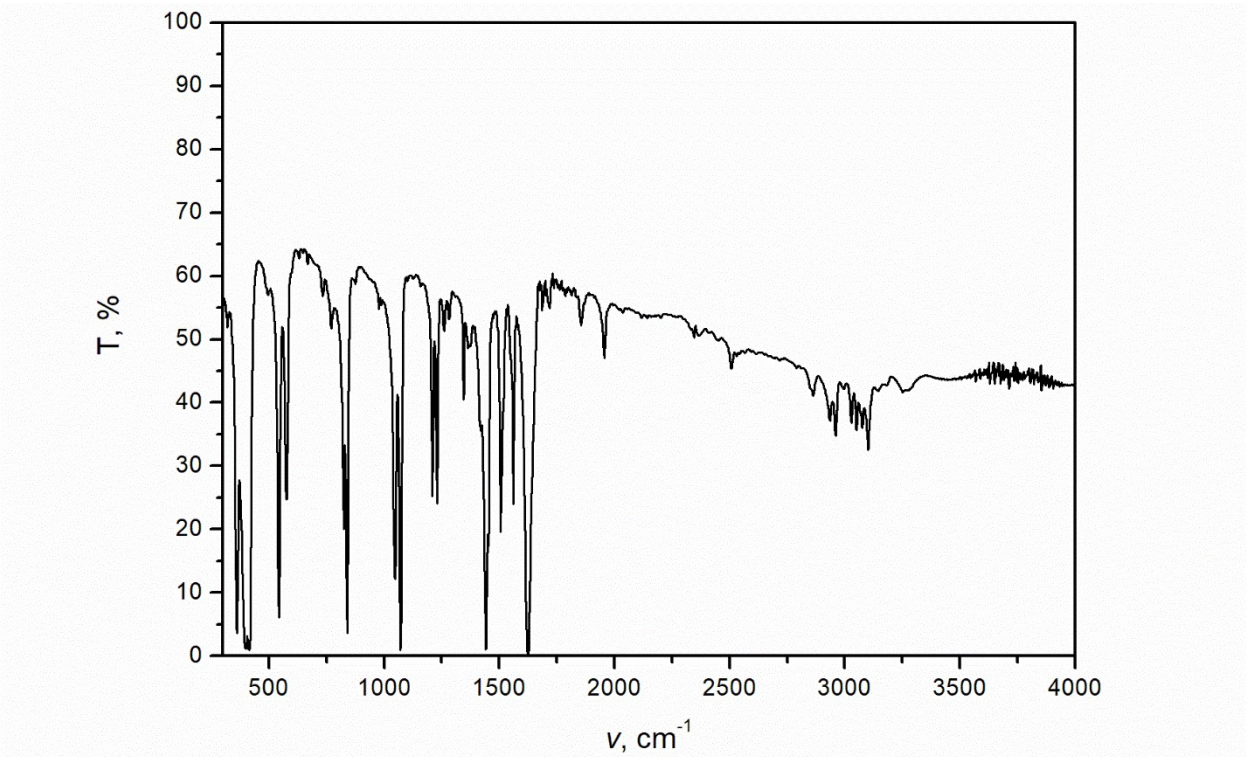


Fig. S17 IR spectrum of **7**.

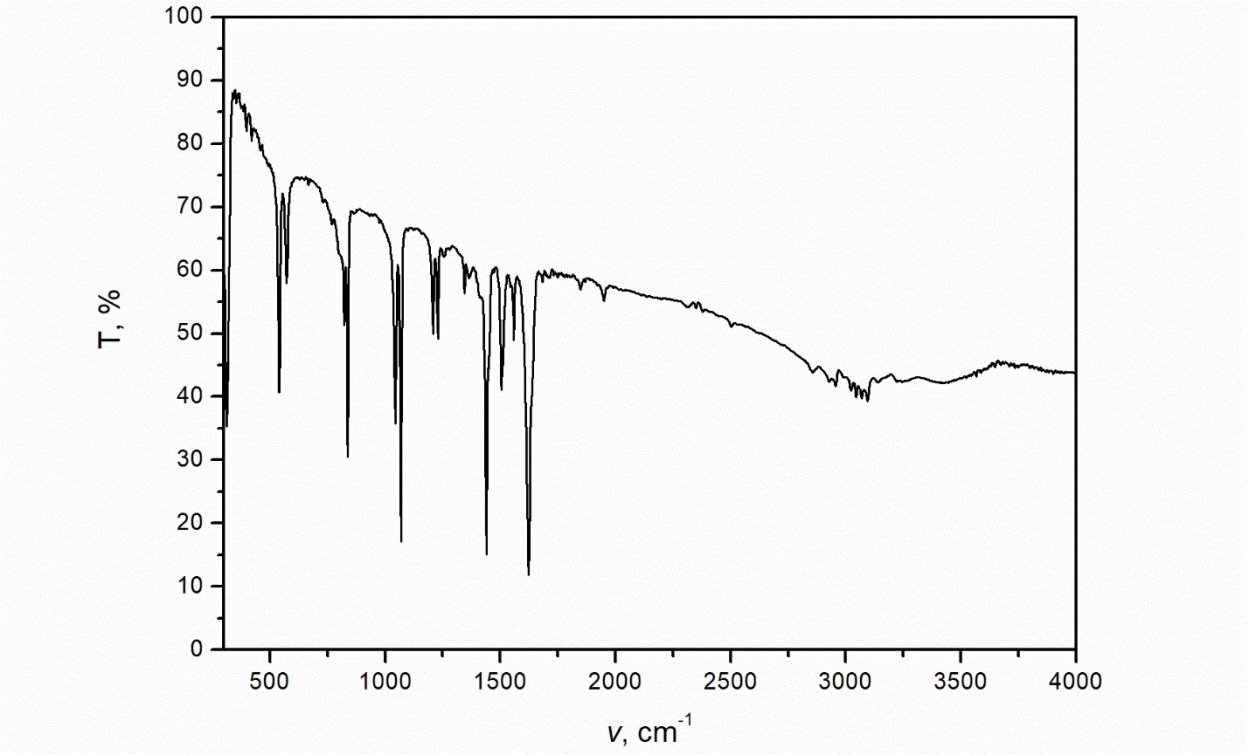


Fig. S18 IR spectrum of **8**.

Table S1. Mass spectrometry study of the complexes **1**-**3** at 350, 400 and 450 °C (70eV).

Ion (X^+)		I/I_0, %								
		1			**2**			**3**		
T, °C		**350**	**400**	**450**	**350**	**400**	**450**	**350**	**400**	**450**
X^+		1.9	1.6	2.1	0.1	3.3	2.8	2.1	4.3	9.9
HX^+		10.3	6.5	8.5	0.4	8.7	5.3	5.1	9.1	18.9
$C_{12}H_{12}N_2^+$		69.2	73.9	71.5	34.0	93.2	75.7	24.9	23.8	31.2
M^+		0.3	0.6	0.9	0.4	16.9	20.5	0.1	0.7	1.2
MX_2^+		3.5	12.2	14.1	1.7	34.7	47.8	0.1	1.2	3.8
MX_3^+		0.2	0.5	0.6	-	3.4	4.6	0.01	0.1	0.2
$MX_2C_6H_6N^+$		2.7	10.2	11.2	0.2	11.0	14.0	0.6	3.3	5.4
$MX_2C_{12}H_{12}N_2^+$		2.8	7.9	7.7	3.1	17.8	25.1	4.2	4.8	6.9
$MX_3C_{12}H_{12}N_2^+$		1.3	3.9	3.7	1.1	2.0	2.4	-	-	-
$M_2X_5C_{12}H_{12}N_2^+$		0.1	0.6	0.7	0.02	2.9	5.6	0.02	0.01	0.03
bpa fragments, m/z	38-41	9.8	15.8	20.0	5.2	15.7	15.2	6.3	19.7	23.5
	50-52	14.1	23.0	26.4	10.2	19.2	20.6	13.6	24.0	32.4
	63-66	40.5	54.7	60.1	49.1	56.5	61.0	72.2	51.6	68.8
	91-93	100	100	100	100	100	100	100	100	100

Table S2. Mass spectrometry study of the complexes **5**-**8** at 350, 400 and 450 °C (70eV).

Ion (X^+)		I/I_0, %											
		5			**6**			**7**			**8**		
T, °C		**350**	**400**	**450**	**350**	**400**	**450**	**350**	**400**	**450**	**350**	**400**	**450**
X^+		3.8	2.3	1.2	32.4	12.9	15.4	2.9	1.5	0.8	7.7	12.3	10.8
HX^+		20.6	13.4	7.0	80.1	31.6	34.5	16.6	7.4	2.9	7.7	9.9	7.4
$C_{12}H_{12}N_2^+$		100	100	100	100	100	100	100	100	100	100	75.5	45.2
M^+		1.2	0.8	0.5	0.8	1.0	1.9	1.2	2.6	3.2	8.2	14.7	12.8
MX_2^+		3.8	7.3	15.7	0.7	9.5	47.6	4.7	18.5	23.0	33.1	100	100
MX_3^+		0.4	1.1	2.2	0.1	0.7	7.3	0.6	3.2	3.7	7.4	21.9	23.9
$MX_2C_6H_6N^+$		7.7	28.2	66.7	2.2	19.6	94.8	1.9	9.9	14.2	22.7	32.8	27.5
$MX_2C_{12}H_{12}N_2^+$		7.3	23.6	49.3	4.8	27.4	94.0	3.9	19.2	24.0	23.1	62.9	71.3
$MX_3C_{12}H_{12}N_2^+$		3.5	6.0	6.3	-	-	0.04	0.5	2.1	2.4	0.1	0.02	0.01
$M_2X_5C_{12}H_{12}N_2^+$		1.5	11.4	24.2	0.02	1.5	12.6	0.3	1.5	2.8	0.1	0.5	0.8
bpa fragments, m/z	38-41	15.4	9.9	7.9	14.2	13.6	17.4	10.8	5.5	4.4	20.6	12.9	7.3
	50-52	14.3	9.5	9.1	11.0	11.2	14.6	7.0	4.7	4.5	12.8	11.2	7.3
	63-66	33.9	26.3	29.6	28.4	29.1	39.0	20.3	16.4	16.9	31.7	30.7	21.4
	91-93	68.1	53.8	56.3	70.0	69.8	81.0	54.4	42.3	41.6	73.1	64.8	45.0

Intermolecular interactions in **1-8**

The packing of molecules and ions in the crystals of **1-8** might be additionally influenced by weak hydrogen bonds and/or π…Hal (hal = Cl, Br) interactions. However, in the compounds **1-4** these intermolecular interactions cannot be studied quantitively because of the crystallographic disorder. Analysis of the site occupancy factors and intermolecular distances between different components of the disorder proves that there is no correlation between them. In another words, each of the disorder components 'has enough space' in the crystal that points to the absence of strong non-bonding interactions.

The analysis of the intermolecular contacts in **5-8** reveals some potential hydrogen bonds (Tables S3-S6) and/or π…Hal (Hal = Cl, Br) interactions.

In the compound **5**, there are two types of C(π)…Cl contacts of 3.555(2) and 3.562(2) Å. The angles at Cl atoms are of 92.82(4) and 155.27(4)°, respectively (Fig. S19a). As a result, the molecules are joined to each other into the infinite layers (1 0 2) (Fig. S19b).

Table S3. Selected hydrogen-bond parameters in compound **5**

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C1—H1···Cl3	0.95	2.98	3.4587 (18)	112.3
C2—H2···Cl1^{i}	0.95	2.90	3.6687 (18)	138.3
C4—H4···Cl1^{ii}	0.95	2.89	3.7815 (17)	156.1
C5—H5···Cl1	0.95	2.91	3.4502 (16)	117.3

Symmetry code(s): (i) *x*, -*y*+3/2, *z*-1/2; (ii) -*x*, *y*+1/2, -*z*+1/2.

Table S4. Selected hydrogen-bond parameters in compound **6**

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C1—H1···Br1	0.95	3.00	3.528 (3)	116.6
C1—H1···Br1^{i}	0.95	2.97	3.643 (3)	129.5
C5—H5···Br3	0.95	2.94	3.500 (3)	118.7

Table S5. Selected hydrogen-bond parameters in compound **7**

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C1—H1···Cl1	0.95	2.93	3.4470 (14)	115.3
C1—H1···Cl1^{i}	0.95	2.82	3.5107 (14)	130.2
C5—H5···Cl2^{ii}	0.95	2.83	3.6445 (15)	144.9
C5—H5···Cl3	0.95	2.91	3.4518 (15)	117.2

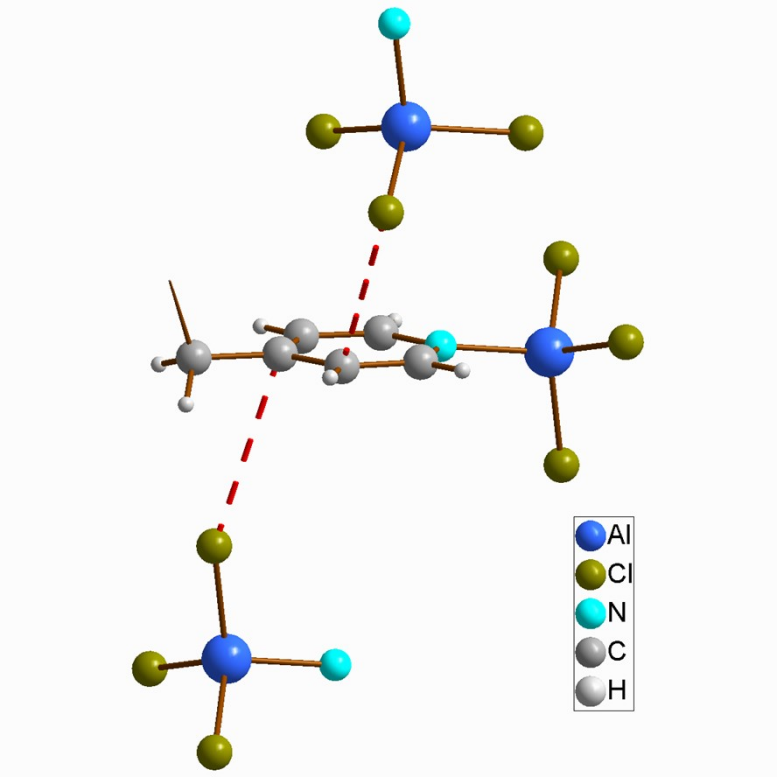
Symmetry code(s): (i) -*x*+2, *y*-1/2, -*z*+1/2; (ii) *x*-1, *y*, *z*.

Table S6. Selected hydrogen-bond parameters in compound **8**

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C1—H1···Br1	0.95	3.00	3.543 (4)	117.4
C1—H1···Br1^{i}	0.95	2.96	3.640 (4)	129.2
C5—H5···Br2^{ii}	0.95	3.00	3.821 (4)	145.1
C5—H5···Br3	0.95	2.97	3.533 (4)	119.4

Symmetry code(s): (i) -*x*+2, *y*-1/2, -*z*+1/2; (ii) *x*-1, *y*, *z*.

a)



b)

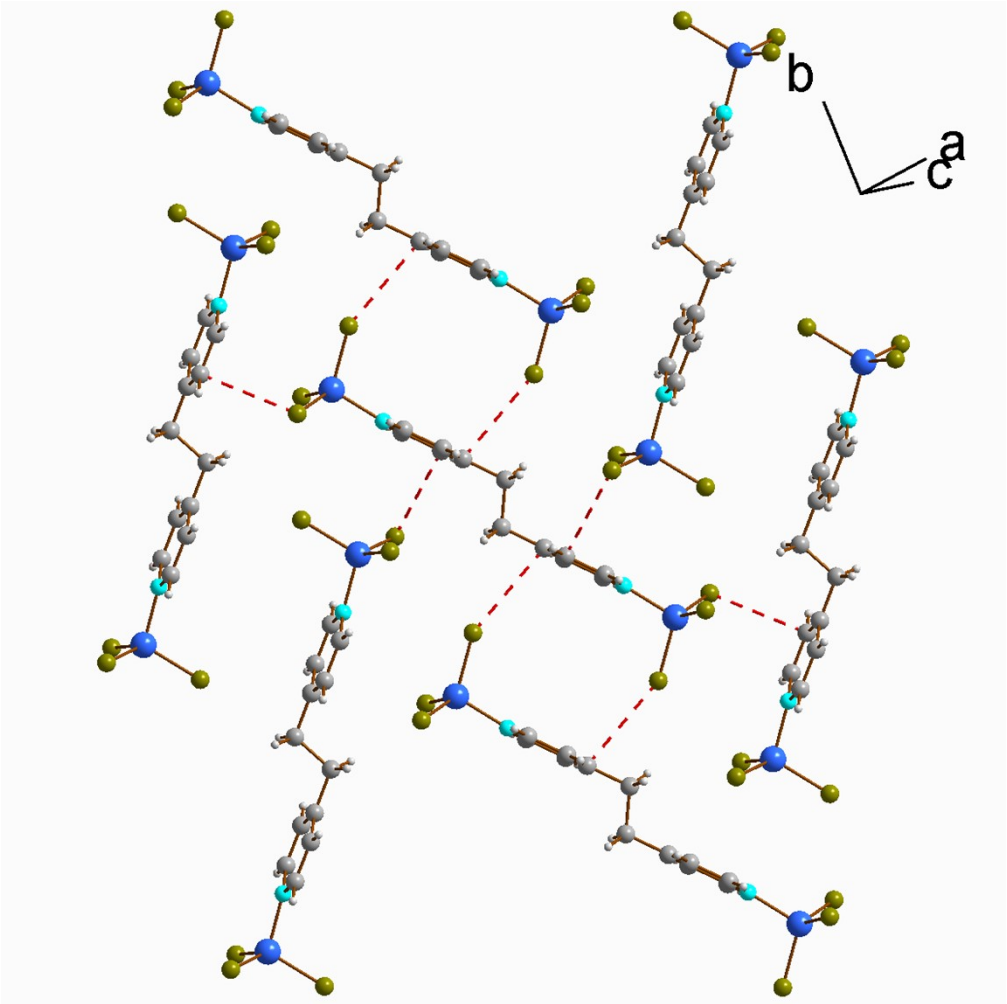


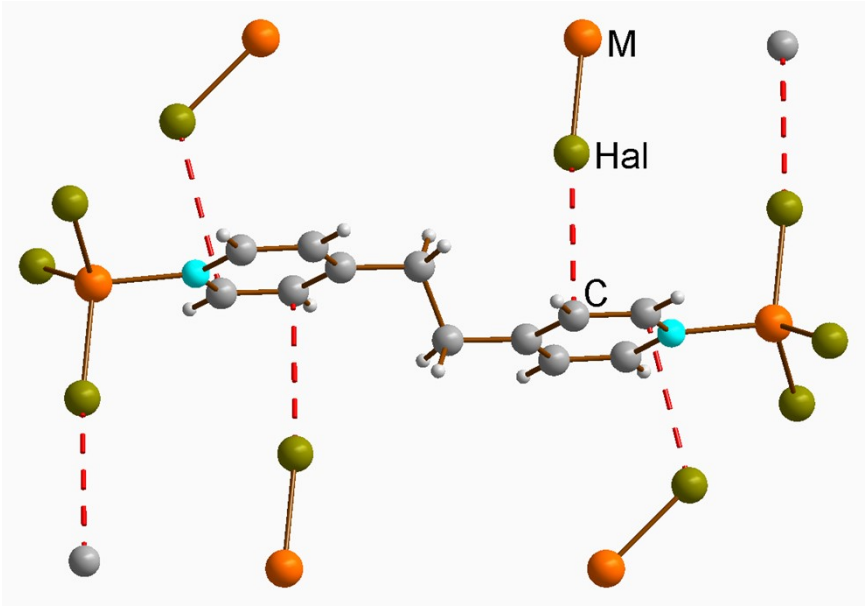
Fig. S19 a) Close-up to the short C…Cl contacts of 3.555(2) and 3.562(2) Å; b) the (1 0 2) layer in the crystal of **5**. Contacts are shown as red dashed lines.

In the isostructural compounds **6**, **7** and **8,** analysis of the intermolecular contacts reveals two types of Hal…C(π) contacts (Fig.S20a, Table S7). These contacts join the molecules into the 3D network (Fig. S20b).

Table S7. Intermolecular Hal…C(π) contacts in compounds **6-8**

Compound	**6**	**7**	**8**
Hal(3)…C(5), Å	3.462(2)	3.3136(13)	3.439(4)
∠M-Hal…C, °	132.18(5)	121.57(3)	122.33(7)
Hal(1)…C(4), Å	3.561(3)	3.4935(14)	3.517(4)
∠M-Hal…C, °	161.19(5)	167.14(3)	169.47(6)

a)



b)

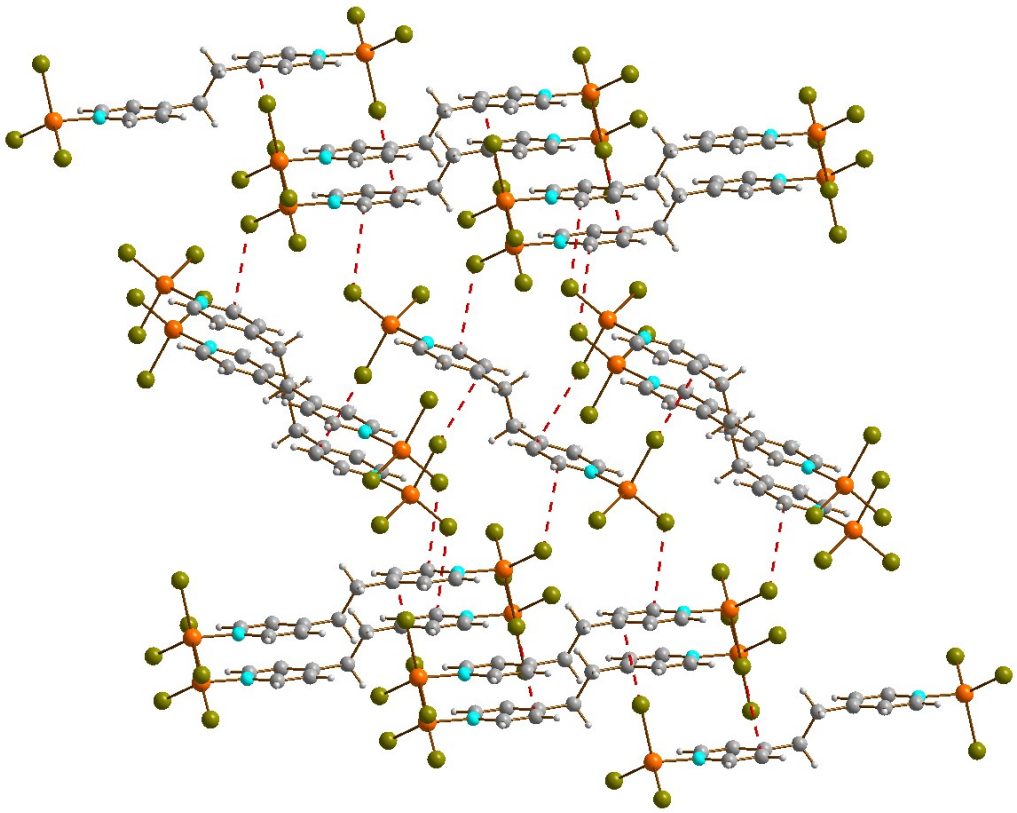


Fig. S20. a) Nearest environment of the molecules **6-8** in the crystal; b) 3D-network based on the C…Hal contacts that are shown as red dashed lines.

Modulation in the crystal structure of compound 3.

The structure of $[AlBr_2(bpa)_2]^+Br$ is modulated, in which the entire polymer chain and/or the positions of the Br- ligands are displaced according to the harmonic law. The diffraction data were obtained on P11 beamline at PETRA III synchrotron, DESY, Hamburg. Diffraction measurements were done at T = 80 K using the radiation with the energy of 18 keV (λ = 0.6888 Å) and Dectris Pilatus 6M photon counting detector. Narrow (0.1°) scans were used to collect 3600 frames by full rotation around the horizontal axis. First 2000 frames were processed using *CrysAlisPro* software package (Rigaku OD), the rest frames were discarded because they were affected by the radiation damage.

The reciprocal lattice reconstruction shows the presence of weak reflections that cannot be indexed in the primitive monoclinic unit cell a=11.77, b=9.74, c=11.57 Å, β = 107.93°, V=1262 Å3. Their *hkl* indices correspond to the ±n/3 series, pointing the harmonic modulation with the vectors of (2/3; 2/3; 1/3) and (1/3; 2/3; 1/3) (Fig. S21).

The sections of the reciprocal space prove this assumption (Fig. S22).

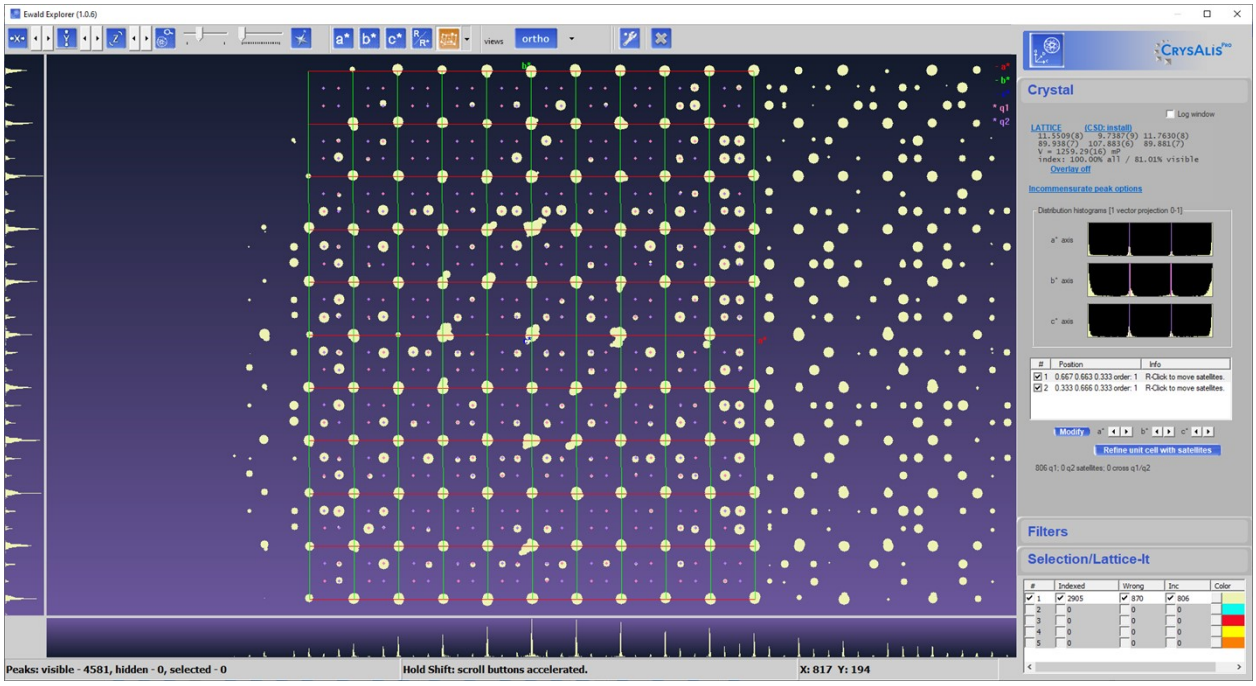


Fig. S21. The reciprocal lattice reconstruction done with *Ewald Explorer* (*CrysAlisPro* software package).

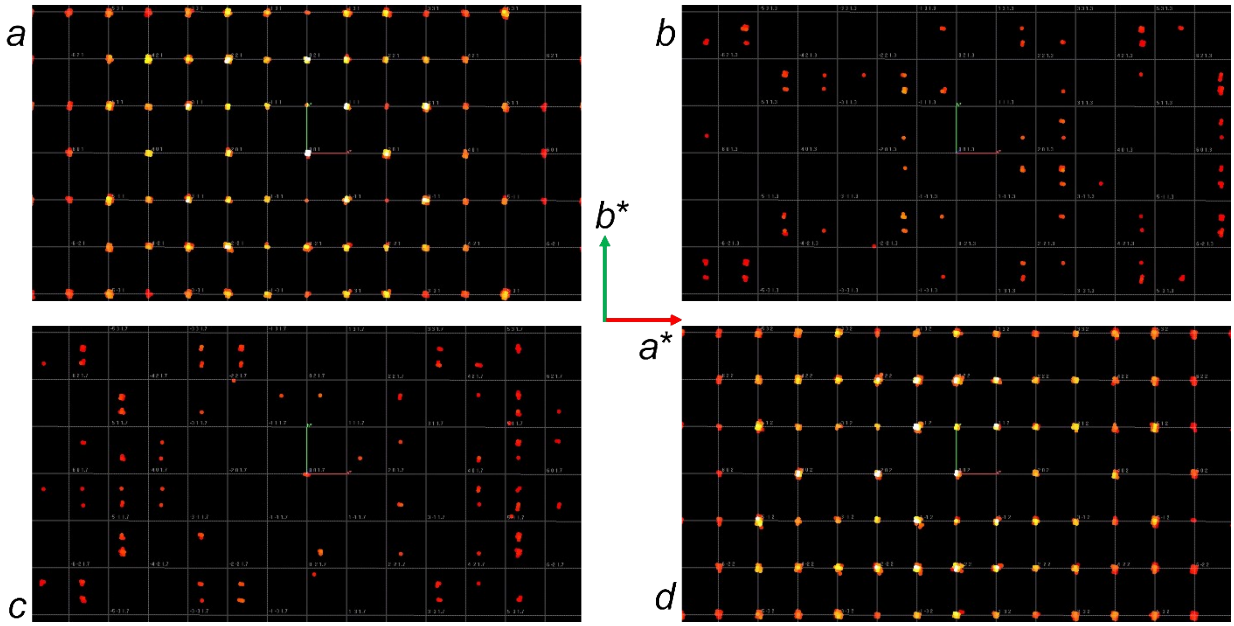
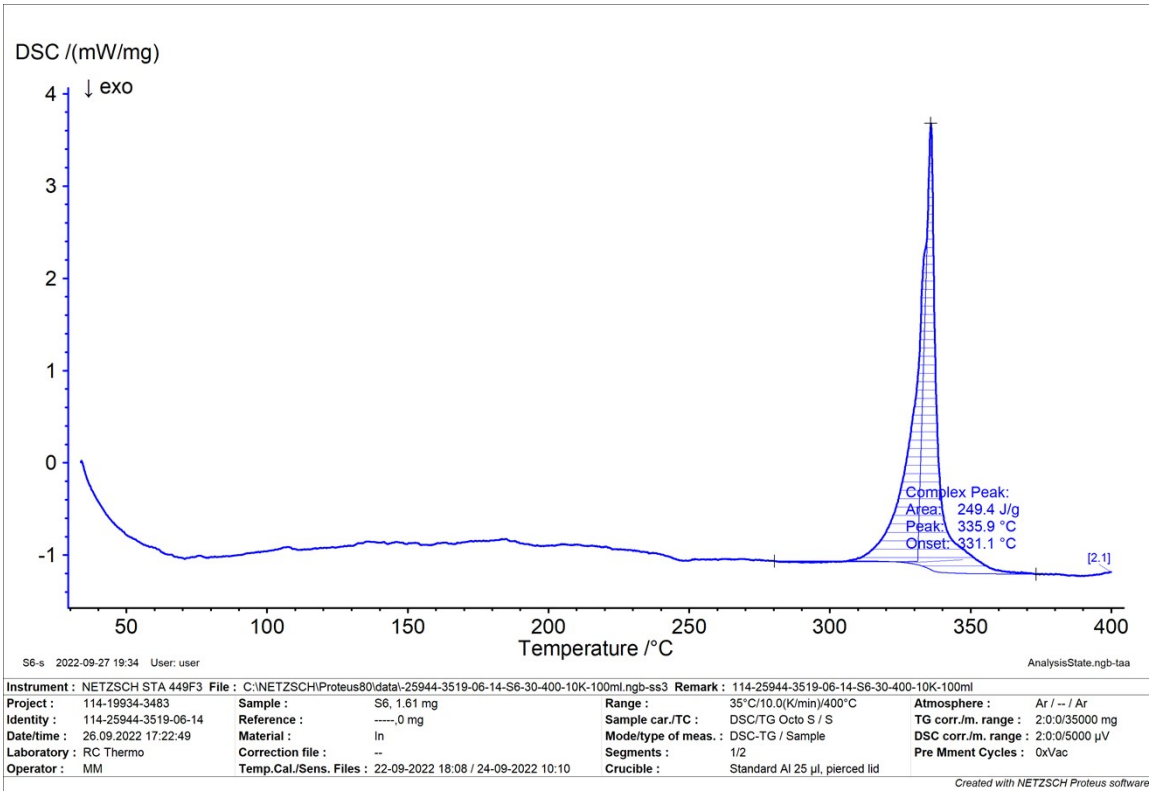


Fig. S22. Layers hkl in the reciprocal space for l = 1 (a), 1.333 (b), 1.667 (c) and 2 (d), generated with the *Ewald3D* (*CrysAlisPro* software package).

However, the intensities of the satellite reflections are so low and cannot be measured at the satisfactory level of I/σ even with the usage of high-flux synchrotron radiation. Therefore, we decided to limit ourselves with the refinement of the average structure. The modulation effect manifests itself in the disorder of terminal Br atoms and relatively large atomic displacement parameters of all non-hydrogen atoms (Fig. 2a in the main text of the article).

a)



b)

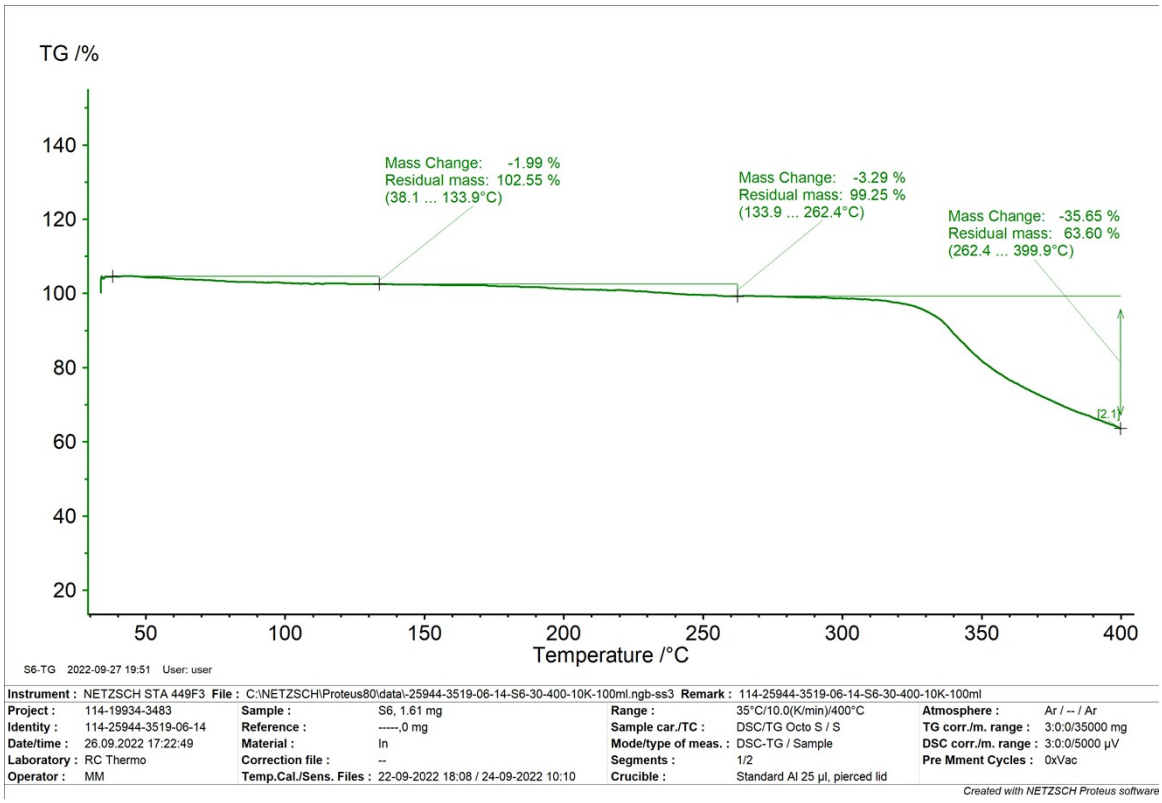
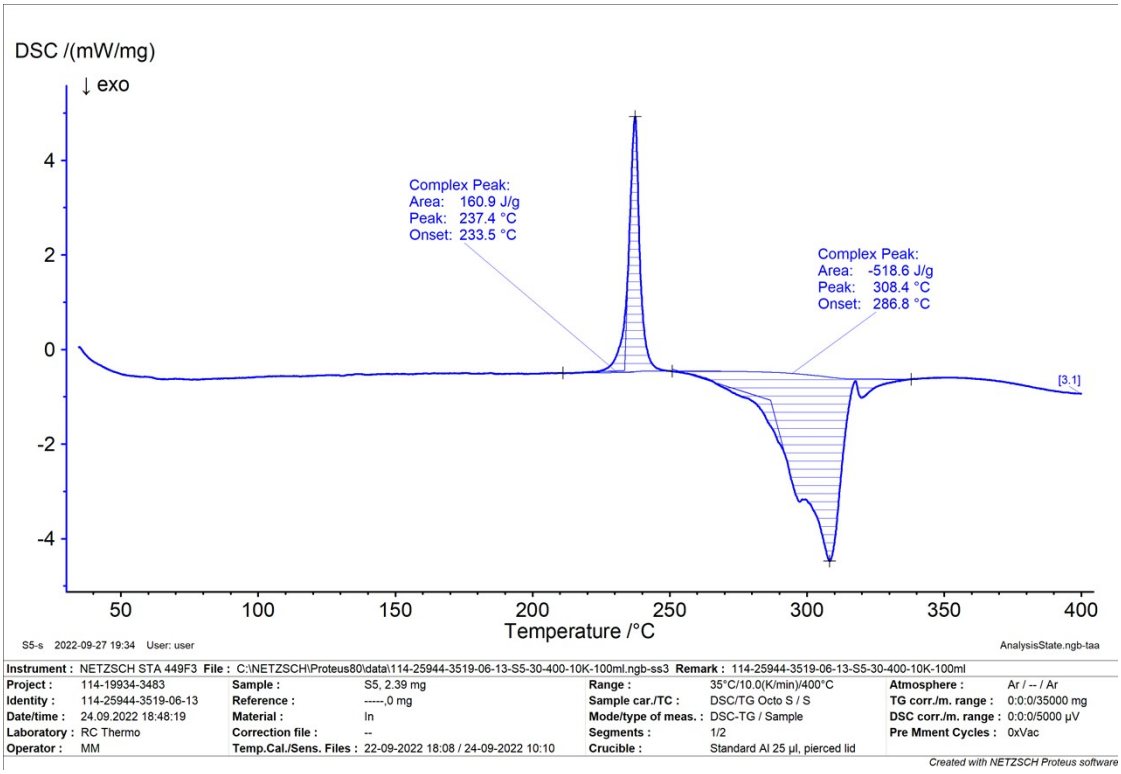


Fig. S23. Simultaneous DSC (a) and TG (b) analysis of **1** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

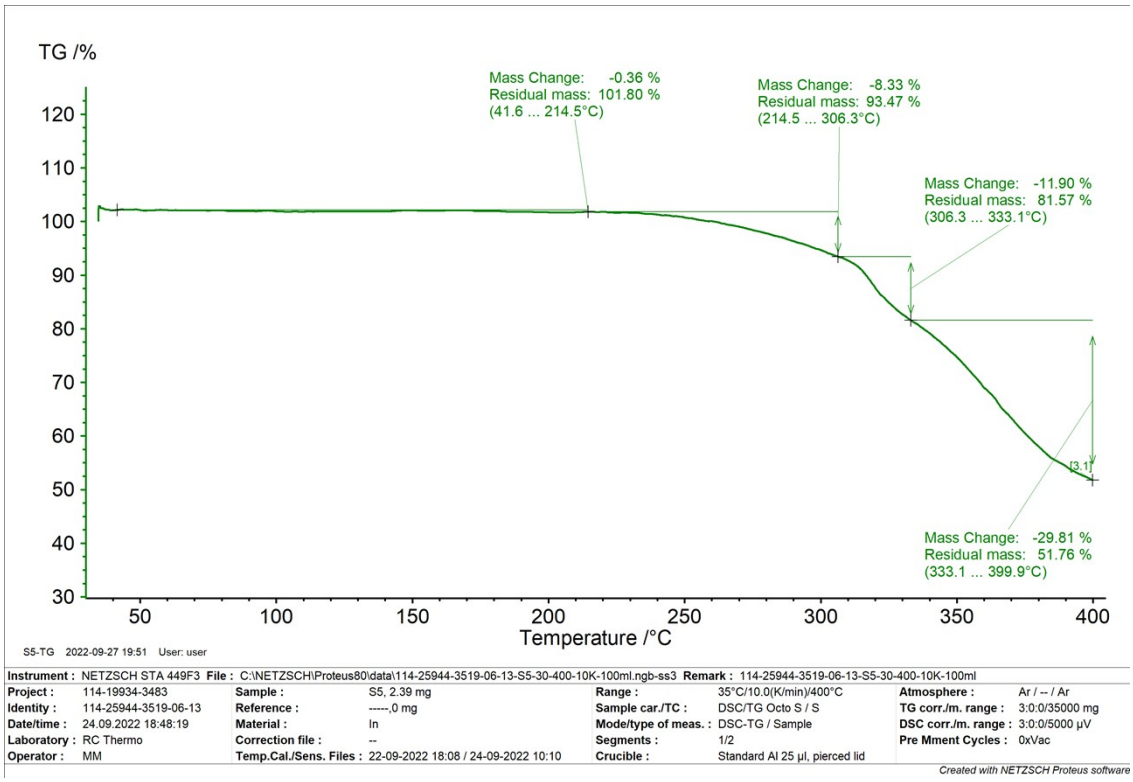
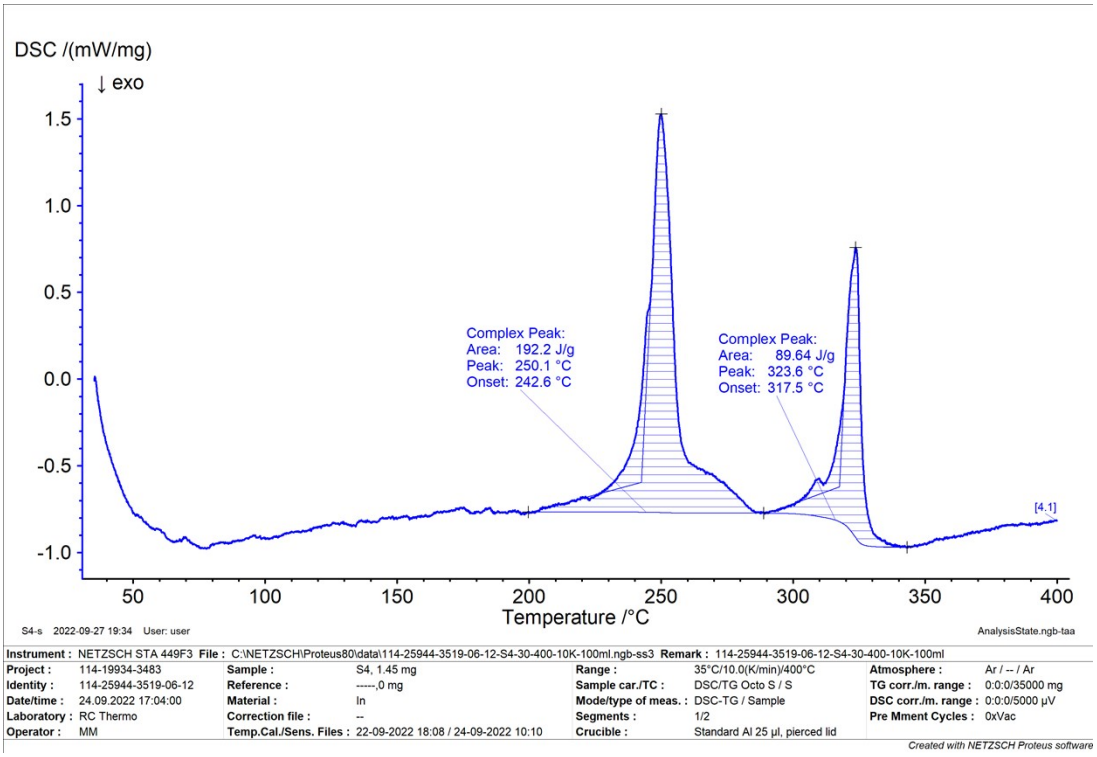


Fig. S24. Simultaneous DSC (a) and TG (b) analysis of **2** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

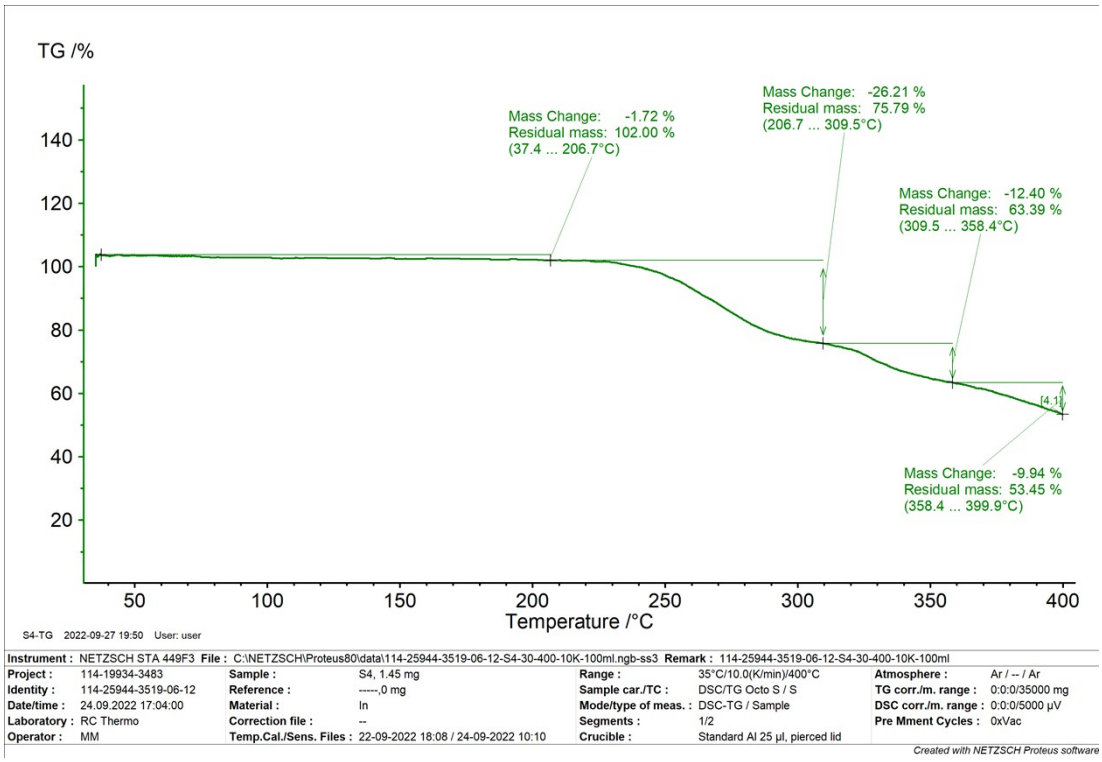
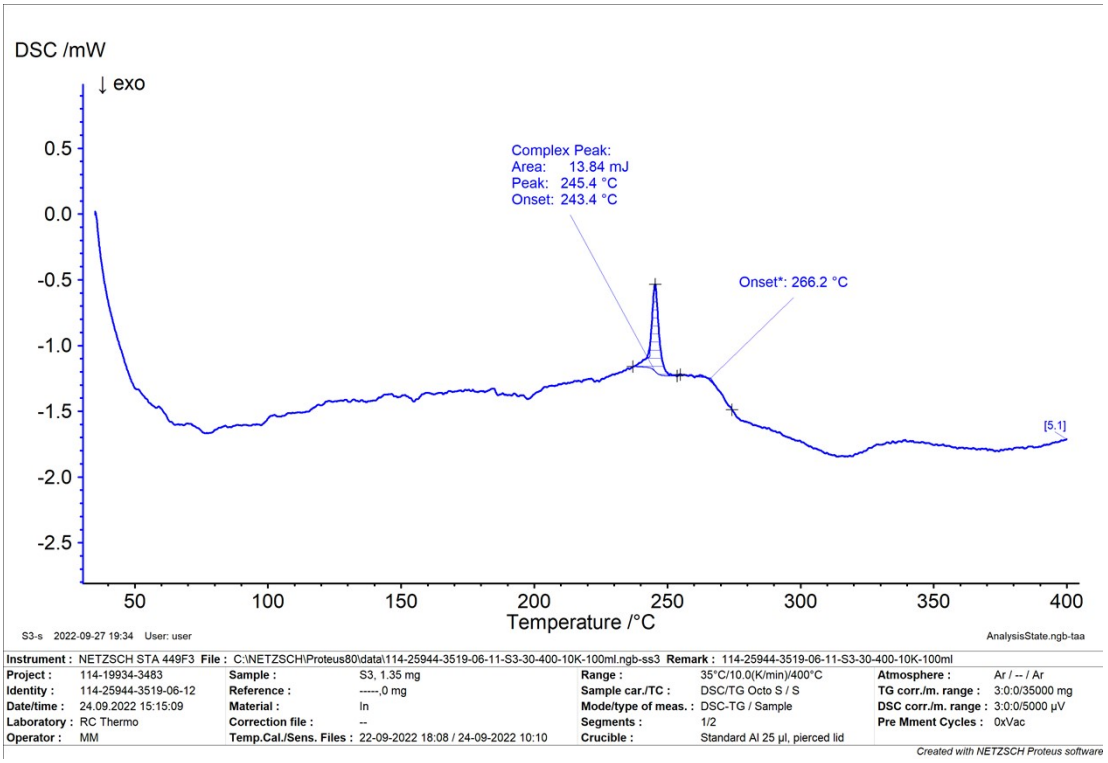


Fig. S25. Simultaneous DSC (a) and TG (b) analysis of **3** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

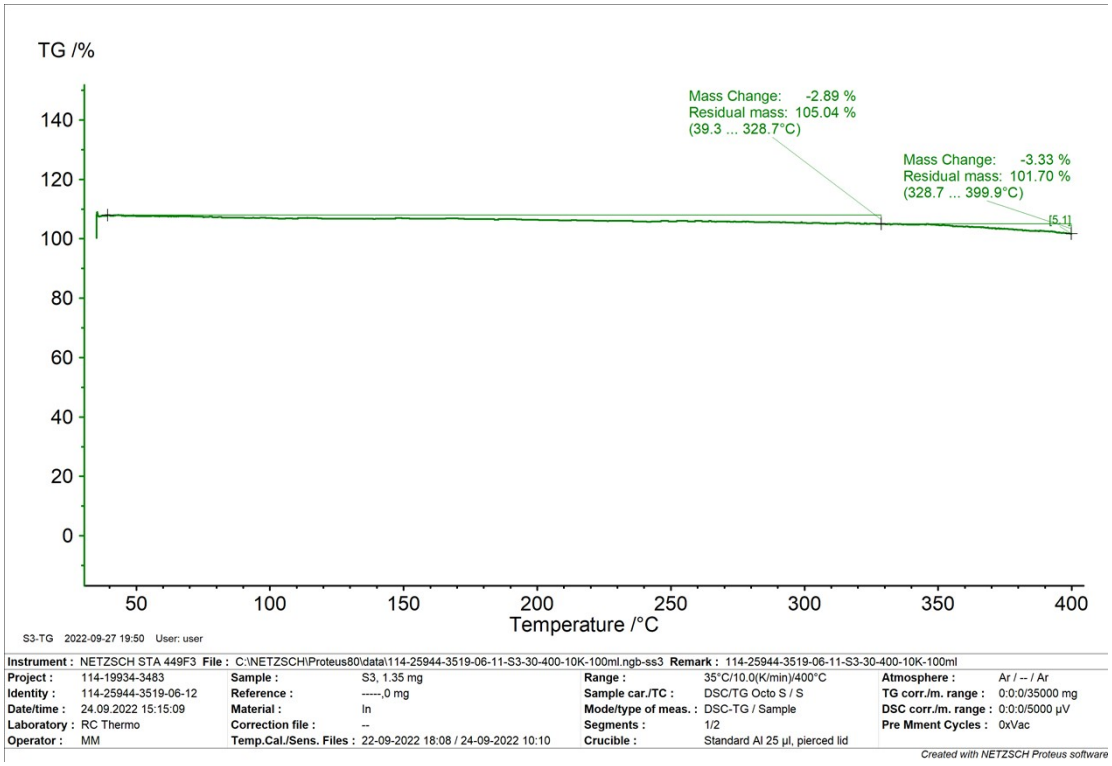
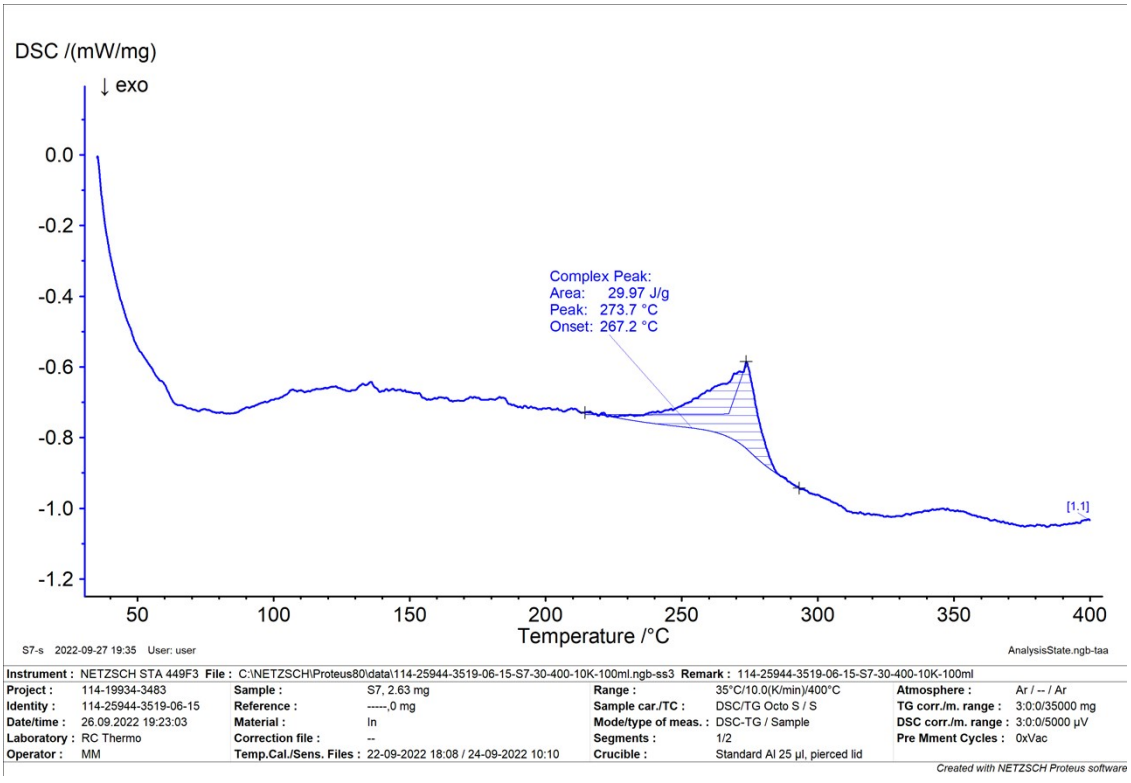


Fig. S26. Simultaneous DSC (a) and TG (b) analysis of **5** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

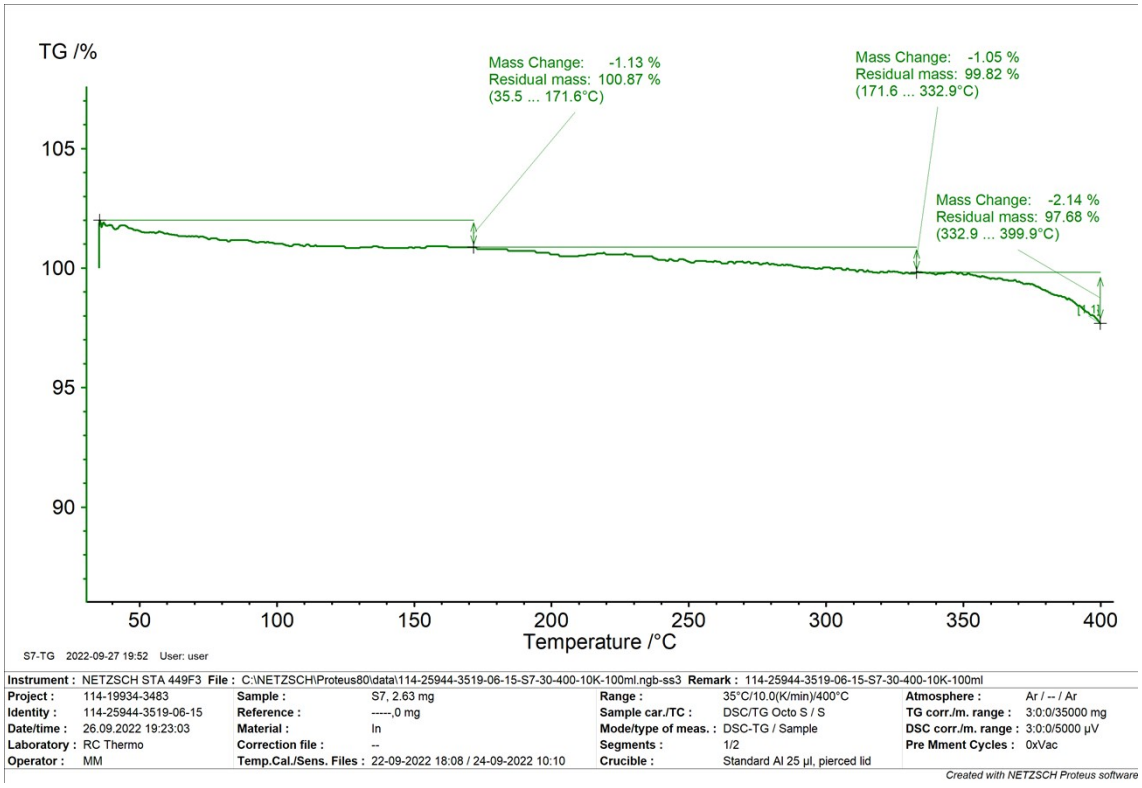
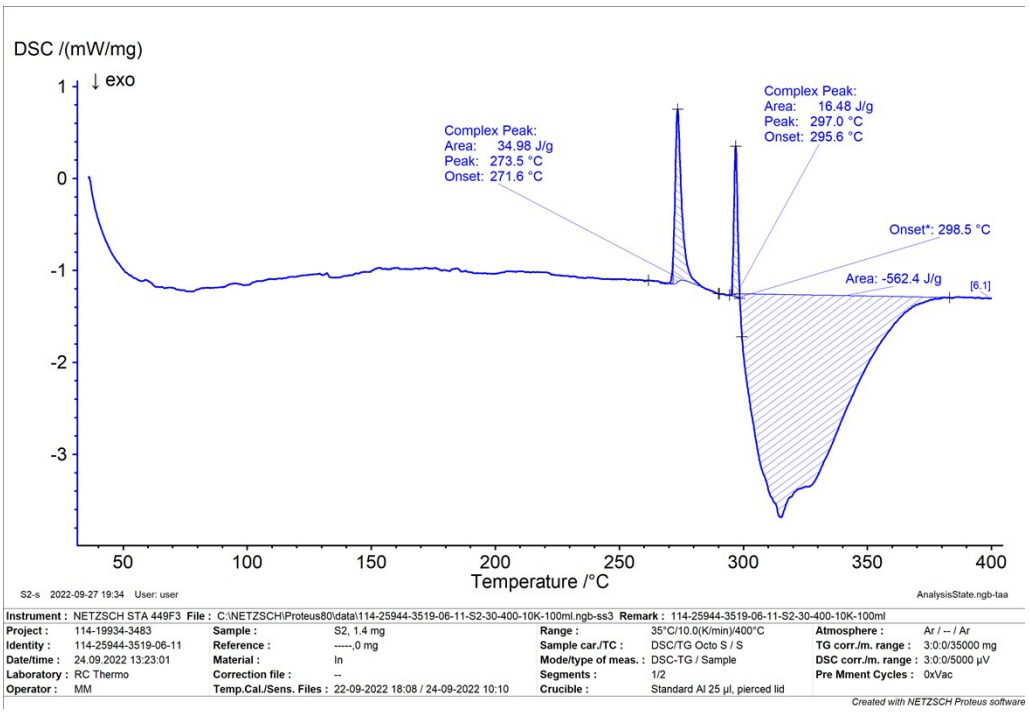


Fig. S27. Simultaneous DSC (a) and TG (b) analysis of **6** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

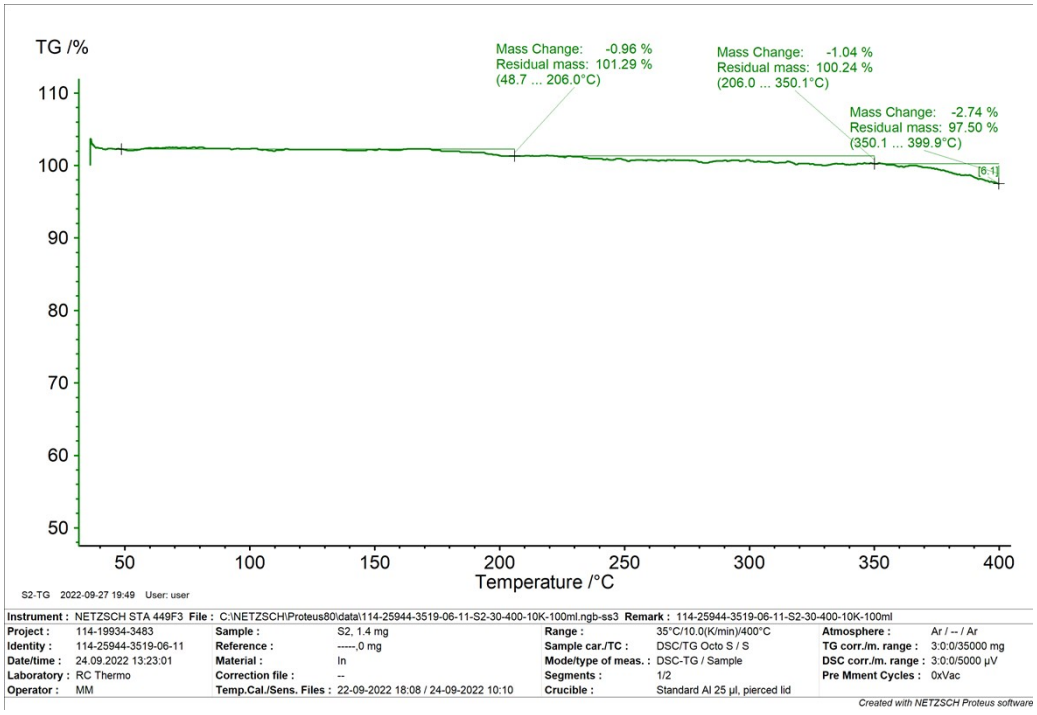
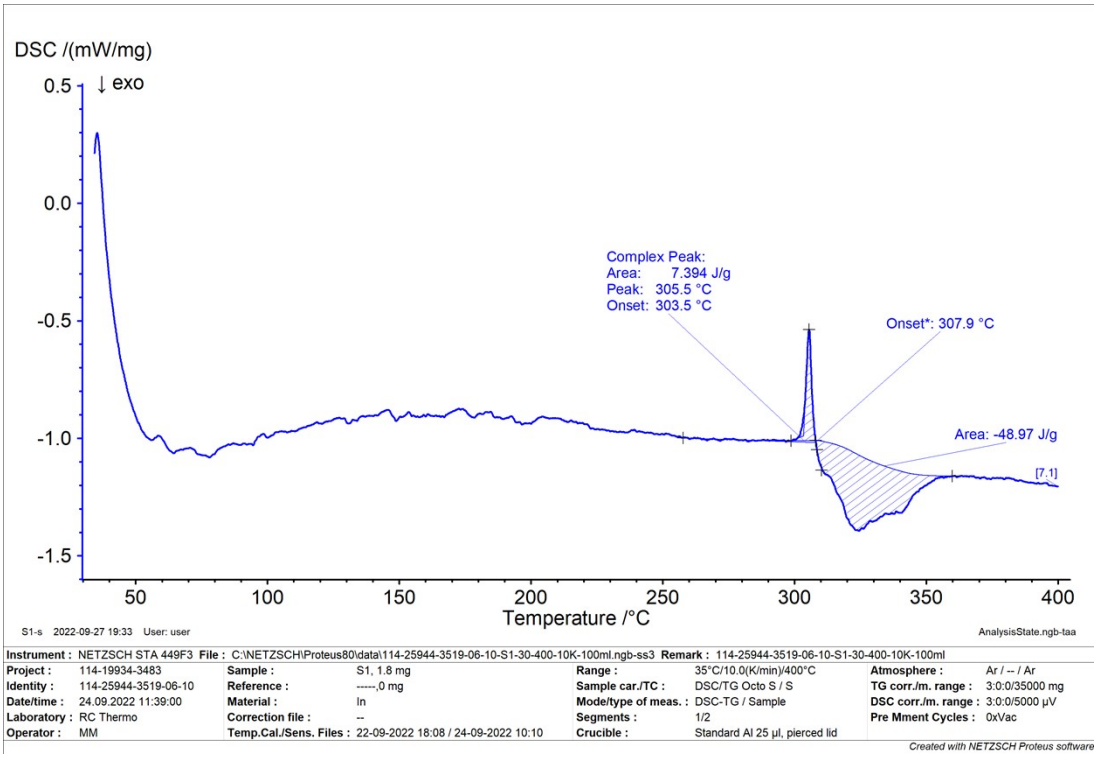


Fig. S28. Simultaneous DSC (a) and TG (b) analysis of **7** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

a)



b)

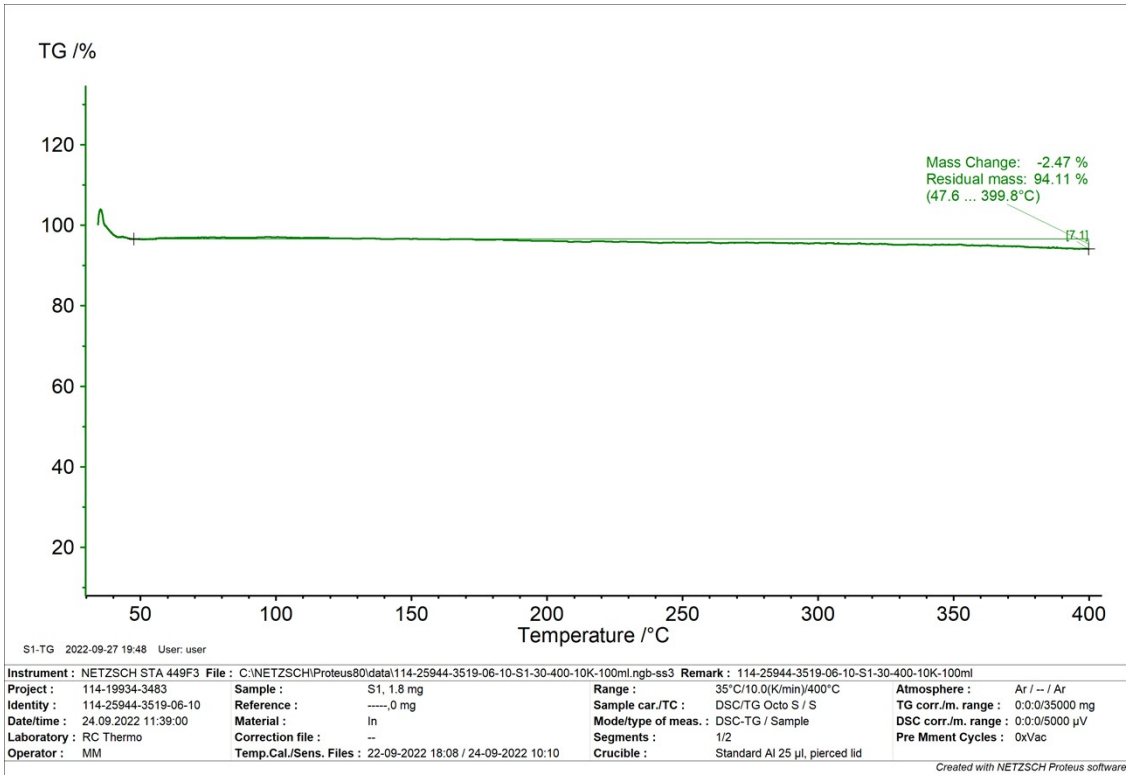


Fig. S29. Simultaneous DSC (a) and TG (b) analysis of **8** in a constant argon flow with a heating rate of 10 K/min from 35 to 400 °C.

Computational data

Table S8. Total energies E_0, standard enthalpies H^o_{298} (in Hartree) and standard entropies S^o_{298} (in cal mol^{-1} K^{-1}) for studied compounds. M06-2X/def2-TZVPPD level of theory.

Compound	E_0	H^o_{298}	S^o_{298}
H^+	0	0.002360	26.014
pyz	-264.4198205	-264.222899	65.443
$pyzH^+$	-264.648695	-264.552269	67.258
$pyzH_2^{2+}$	-264.8084612	-264.699043	66.079
bipy	-495.3547432	-495.185749	89.736
$bipyH^+$	-495.7205761	-495.537634	91.583
$bipyH_2^{2+}$	-495.9813436	-495.784534	90.807
bpe	-572.7502557	-572.545324	106.254
$bpeH^+$	-573.1228687	-572.903904	109.884
$bpeH_2^{2+}$	-573.4074809	-573.174417	105.880
bpa	-573.9702118	-573.741267	109.872
$bpaH^+$	-574.3393886	-574.096334	111.157
$bpaH_2^{2+}$	-574.6320422	-574.374741	111.043

Table S9. Total energies E_0, standard enthalpies H^o_{298} (in Hartree) and standard entropies S^o_{298} (in cal mol^{-1} K^{-1}) for studied compounds. M06-2X/def2-TZVP level of theory.

Compound	E_0	H^o_{298}	S^o_{298}
pyz	-264.3030778	-264.220400	65.403
bipy	-495.3502448	-495.181216	89.852
bpe	-572.7447279	-572.53976	112.221
bpa	-573.9640089	-573.735068	111.016
$AlCl_3$	-1623.236421	-1623.225297	74.733
$AlBr_3$	-7965.213645	-7965.203144	83.138
$GaCl_3$	-3305.62567	-3305.615112	77.715
$GaBr_3$	-9647.616848	-9647.606823	86.056
$(AlCl_3)_2$(pyz) (C_{2h})	-3510.88740650	-3510.777198	145.073
$(AlBr_3)_2$(pyz) (C_i)	-16194.8387481	-16194.729781	161.546
$(GaCl_3)_2$(pyz) (C_{2h})	-6875.6502852	-6875.541418	152.316
$(GaBr_3)_2$(pyz) (C_i)	-19559.6273145	-19559.519564	170.517
$AlCl_3$pyz (C_1)	-1887.601499	-1887.504738	105.769
$AlBr_3$pyz (C_1)	-8229.577658	-8229.481581	113.957
$GaCl_3$pyz (C_s)	-3569.982173	-3569.886207	111.01
$GaBr_3$pyz (C_1)	-9911.970901	-9911.875387	117.387
$(AlCl_3)_2$(bipy) (C_2)	-3741.9550197	-3741.758069	169.174
$(AlBr_3)_2$(bipy) (C_2)	-16425.9067631	-16425.710976	184.546
$(GaCl_3)_2$(bipy) (C_2)	-7106.7169266	-7106.521293	176.992
$(GaBr_3)_2$(bipy) (C_2)	-19790.6937088	-19790.499144	191.008
$AlCl_3$bipy (C_1)	-2118.655221	-2118.472107	132.043
$AlBr_3$bipy (C_1)	-8460.631536	-8460.449018	138.914
$GaCl_3$bipy (C_1)	-3801.035681	-3800.853278	135.522
$GaBr_3$bipy (C_1)	-10143.02435	-10142.84245	142.641
$(AlCl_3)_2$(bpe) (C_2)	-3819.3538386	-3819.120701	182.954
$(AlBr_3)_2$(bpe) (C_2)	-16503.3056829	-16503.073666	199.982
$(GaCl_3)_2$(bpe) (C_2)	-7184.1155355	-7183.883809	193.633
$(GaBr_3)_2$(bpe) (C_2)	-19868.0922369	-19867.861507	209.515
$AlCl_3$bpe (C_1)	-2196.051316	-2195.832072	143.363
$AlBr_3$bpe (C_1)	-8538.027692	-8537.809033	150.966
$GaCl_3$bpe (C_1)	-3878.431677	-3878.213115	147.809
$GaBr_3$bpe (C_1)	-10220.42038	-10220.20234	155.256
$(AlCl_3)_2$(bpa) (C_i)	-3820.5751489	-3820.317970	189.633
$(AlBr_3)_2$(bpa) (C_i)	-16504.5270901	-16504.271041	203.061
$(GaCl_3)_2$(bpa) (C_i)	-7185.3368607	-7185.081082	196.805
$(GaBr_3)_2$(bpa) (C_i)	-19869.3136580	-19869.058813	210.179
$AlCl_3$bpa (C_1)	-2197.270853	-2197.027616	149.329
$AlBr_3$bpa (C_1)	-8539.247283	-8539.004672	155.78
$GaCl_3$bpa (C_1)	-3879.651277	-3879.407848	153.308
$GaBr_3$bpa (C_1)	-10221.64006	-10221.39798	158.43

Table S10. Thermodynamic data for the gas phase processes of dissociation of MX_3 complexes. Standard reaction enthalpies $\Delta_{diss}H°_{298}$ and Gibbs energies $\Delta_{diss}G°_{298}$ are in kJ mol^{-1}, standard reaction entropies $\Delta_{diss}S°_{298}$ in J mol^{-1} K^{-1}. M06-2X/def2-TZVP level of theory.

Compound	$\Delta_{diss}H°_{298}$	$\Delta_{diss}S°_{298}$	$\Delta_{diss}G°_{298}$
	$(MX_3)_2(pyz) = 2MX_3 + pyz$		
$AlCl_3$	278.8	292.0	191.8
$AlBr_3$	270.7	293.4	183.2
$GaCl_3$	238.4	286.7	153.0
$GaBr_3$	224.5	280.3	141.0
	$(MX_3)_2(pyz) = MX_3pyz + MX_3$		
$AlCl_3$	123.8	148.2	79.7
$AlBr_3$	118.3	148.7	74.0
$GaCl_3$	105.3	152.3	59.9
$GaBr_3$	98.1	137.8	57.0
	$MX_3pyz = MX_3 + pyz$		
$AlCl_3$	155.0	143.8	112.2
$AlBr_3$	152.4	144.7	109.3
$GaCl_3$	133.1	134.3	93.1
$GaBr_3$	126.5	142.6	84.0
	$(MX_3)_2(bipy) = 2MX_3 + bipy$		
$AlCl_3$	331.5	293.5	244.0
$AlBr_3$	324.2	299.5	234.9
$GaCl_3$	288.4	285.7	203.3
$GaBr_3$	273.8	296.9	185.3
	$(MX_3)_2(bipy) = MX_3bipy + MX_3$		
$AlCl_3$	159.3	157.3	112.4
$AlBr_3$	154.4	156.9	107.7
$GaCl_3$	138.9	151.6	93.7
$GaBr_3$	130.9	157.7	83.9
	$MX_3bipy = MX_3 + bipy$		
$AlCl_3$	172.2	136.2	131.6
$AlBr_3$	169.8	142.6	127.3
$GaCl_3$	149.5	134.1	109.6
$GaBr_3$	142.9	139.2	101.4

Compound	$\Delta_{diss}H°_{298}$	$\Delta_{diss}S°_{298}$	$\Delta_{diss}G°_{298}$
	$(MX_3)_2(bpe) = 2MX_3 + bpe$		
$AlCl_3$	342.2	329.4	244.1
$AlBr_3$	335.1	328.5	237.2
$GaCl_3$	298.8	309.7	206.6
$GaBr_3$	283.8	313.0	190.5
	$(MX_3)_2(bpe) = MX_3bpe + MX_3$		
$AlCl_3$	166.3	147.0	122.5
$AlBr_3$	161.4	142.8	118.9
$GaCl_3$	145.9	133.4	106.2
$GaBr_3$	137.4	133.0	97.8
	$MX_3bpe = MX_3 + bpe$		
$AlCl_3$	175.9	182.4	121.6
$AlBr_3$	173.6	185.7	118.3
$GaCl_3$	152.9	176.3	100.4
$GaBr_3$	146.4	180.0	92.8
	$(MX_3)_2(bpa) = 2MX_3 + bpa$		
$AlCl_3$	347.4	291.2	260.6
$AlBr_3$	340.5	305.3	249.5
$GaCl_3$	304.0	286.1	218.7
$GaBr_3$	289.0	300.0	199.7
	$(MX_3)_2(bpa) = MX_3bpa + MX_3$		
$AlCl_3$	170.8	144.1	127.9
$AlBr_3$	166.0	150.0	121.3
$GaCl_3$	152.6	143.2	109.9
$GaBr_3$	141.8	143.5	99.0
	$MX_3bpa = MX_3 + bpa$		
$AlCl_3$	176.5	147.1	132.7
$AlBr_3$	174.5	155.3	128.2
$GaCl_3$	151.4	142.9	108.8
$GaBr_3$	147.2	156.4	100.6

Table S11. Charge transfer values for $(MX_3)_2(L)$ complexes (per two MX_3 units). M06-2X/def2-TZVP level of theory.

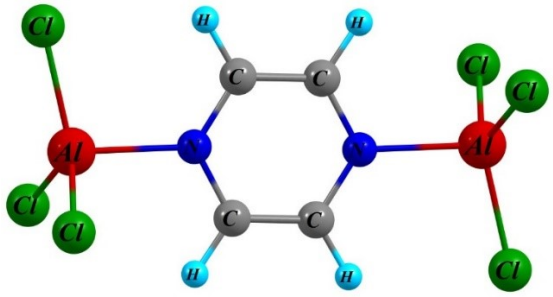
MX_3\L	**pyz**	**bipy**	**bpe**	**bpa**
$AlCl_3$	0.695	0.818	0.843	0.854
$AlBr_3$	0.683	0.818	0.840	0.857
$GaCl_3$	0.525	0.648	0.679	0.691
$GaBr_3$	0.517	0.654	0.677	0.695

Table S12. Charge transfer values for MX_3L complexes (per one MX_3 unit). M06-2X/def2-TZVP level of theory.

MX_3\L	**pyz**	**bipy**	**bpe**	**bpa**
$AlCl_3$	0.408	0.434	0.441	0.439
$AlBr_3$	0.409	0.436	0.443	0.442
$GaCl_3$	0.325	0.351	0.359	0.357
$GaBr_3$	0.326	0.355	0.363	0.363

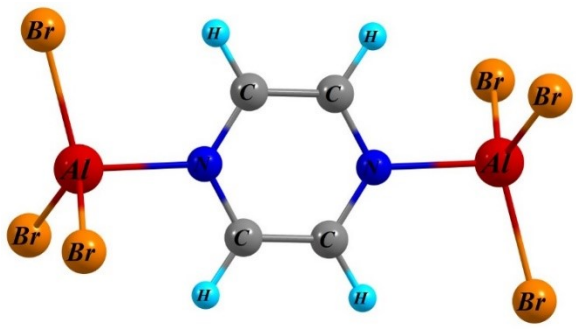
Fig. S30. Optimized structures and xyz coordinates for MX_3 complexes. M06-2X/def2-TZVP level of theory.

$(AlCl_3)_2(pyz)$ (C_{2h})



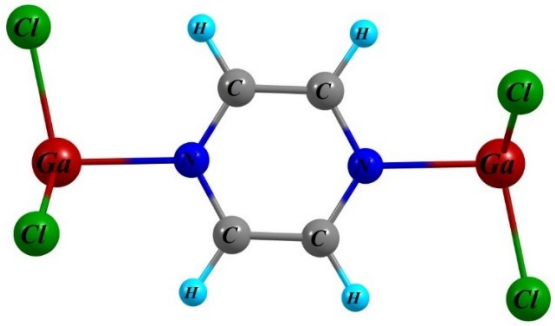
	X	Y	Z
Cl	-3.239540	2.117944	1.774395
Cl	-4.301664	-0.826949	0.000000
Cl	-3.239540	2.117944	-1.774395
Al	-3.239540	0.988430	0.000000
N	-1.318717	0.353455	0.000000
C	-0.369220	1.288662	0.000000
C	0.967833	0.931707	0.000000
H	-0.686761	2.323487	0.000000
H	1.764210	1.663436	0.000000
N	1.318717	-0.353455	0.000000
C	0.369220	-1.288662	0.000000
C	-0.967833	-0.931707	0.000000
H	0.686761	-2.323487	0.000000
H	-1.764210	-1.663436	0.000000
Cl	3.239540	-2.117944	-1.774395
Cl	4.301664	0.826949	0.000000
Cl	3.239540	-2.117944	1.774395
Al	3.239540	-0.988430	0.000000

$(AlBr_3)_2(pyz)$ (C_i)



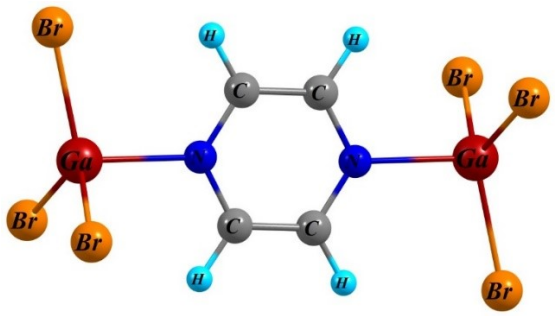
	X	Y	Z
Br	-1.054381	3.204123	2.772623
Br	-3.790912	0.480960	2.438795
Br	-3.153372	3.007595	-0.428590
Al	-2.385375	1.948689	1.428334
N	-0.984499	0.744544	0.587927
C	-0.017973	1.334828	-0.115358
C	0.978878	0.582429	-0.710982
H	-0.047097	2.413661	-0.199579
H	1.775913	1.032187	-1.287442
N	0.984499	-0.744544	-0.587927
C	0.017973	-1.334828	0.115358
C	-0.978878	-0.582429	0.710982
H	0.047097	-2.413661	0.199579
H	-1.775913	-1.032187	1.287442
Br	1.054381	-3.204123	-2.772623
Br	3.790912	-0.480960	-2.438795
Br	3.153372	-3.007595	0.428590
Al	2.385375	-1.948689	-1.428334

$(GaCl_3)_2(pyz)$ (C_{2h})



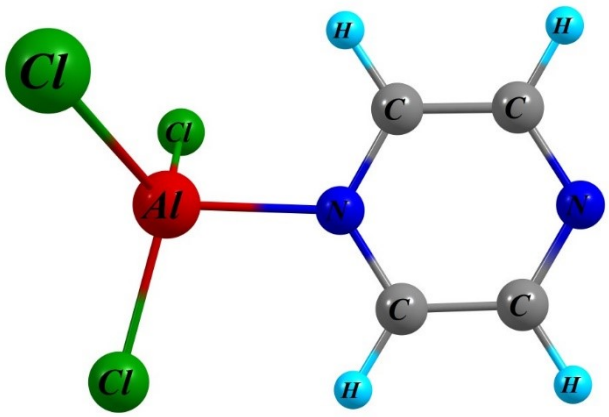
	X	Y	Z
Cl	-3.342491	2.095398	1.826749
Cl	-4.342850	-0.979257	0.000000
Cl	-3.342491	2.095398	-1.826749
Ga	-3.342491	0.937978	0.000000
N	-1.322032	0.326260	0.000000
C	-0.395243	1.281570	0.000000
C	0.949533	0.951112	0.000000
H	-0.734917	2.309668	0.000000
H	1.732709	1.698036	0.000000
N	1.322032	-0.326260	0.000000
C	0.395243	-1.281570	0.000000
C	-0.949533	-0.951112	0.000000
H	0.734917	-2.309668	0.000000
H	-1.732709	-1.698036	0.000000
Cl	3.342491	-2.095398	-1.826749
Cl	4.342850	0.979257	0.000000
Cl	3.342491	-2.095398	1.826749
Ga	3.342491	-0.937978	0.000000

$(GaBr_3)_2(pyz)$ (C_i)



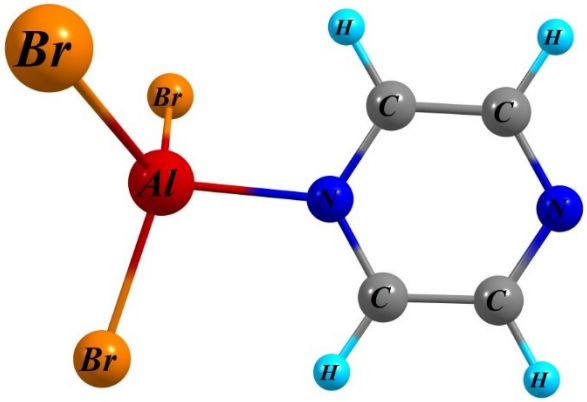
	X	Y	Z
Ga	2.461624	-1.972085	1.479906
Br	1.089010	-3.229094	2.863493
Br	3.856868	-0.406106	2.466985
Br	3.215360	-3.054132	-0.427984
N	0.984494	-0.733958	0.592575
C	0.996787	0.593989	0.675940
C	0.003528	-1.338397	-0.073811
H	1.809471	1.051273	1.225278
H	0.021844	-2.420000	-0.123452
N	-0.984494	0.733958	-0.592575
C	-0.996787	-0.593989	-0.675940
C	-0.003528	1.338397	0.073811
H	-1.809471	-1.051273	-1.225278
H	-0.021844	2.420000	0.123452
Ga	-2.461624	1.972085	-1.479906
Br	-1.089010	3.229094	-2.863493
Br	-3.856868	0.406106	-2.466985
Br	-3.215360	3.054132	0.427984

$AlCl_3pyz$ (C_1)



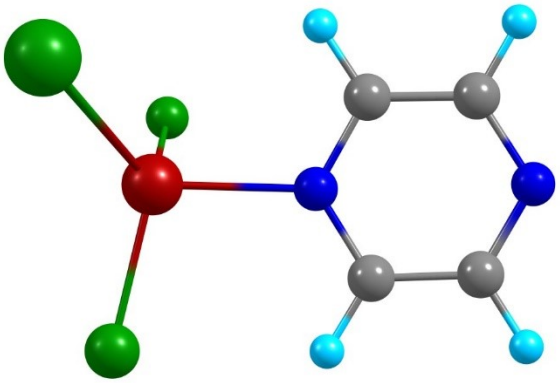
	X	Y	Z
Cl	1.501881	-1.06775	1.773862
Cl	1.671982	2.045458	-0.00395
Cl	1.503386	-1.07562	-1.76882
Al	1.124156	0.009059	-0.00024
N	-0.86719	0.071948	-0.0005
C	-1.52055	-1.093	-0.00025
C	-2.90467	-1.11317	-0.00012
H	-0.9218	-1.99509	-0.00018
H	-3.43973	-2.05427	0.000026
N	-3.62398	0.003165	-0.00029
C	-2.96131	1.150767	-0.00054
C	-1.57462	1.201377	-0.00051
H	-3.54157	2.06483	-0.00066
H	-1.01912	2.129646	-0.00058

$AlBr_3pyz$ (C_1)



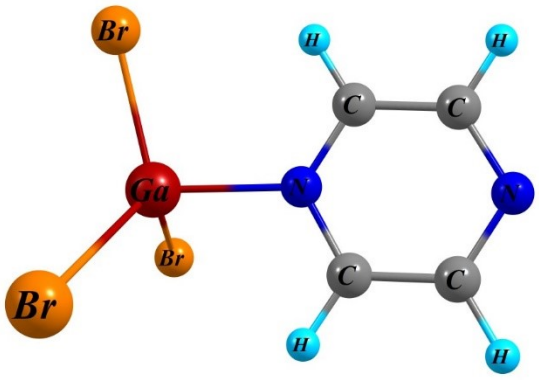
	X	Y	Z
Br	0.853958	-0.9827	2.040902
Br	1.294545	2.14503	-0.18622
Br	0.999237	-1.36655	-1.76622
Al	0.566464	-0.00307	0.005628
N	-1.42297	0.145777	-0.06655
C	-2.12874	-0.98928	-0.07662
C	-3.51204	-0.94805	-0.08548
H	-1.57241	-1.91814	-0.0803
H	-4.08738	-1.86492	-0.09321
N	-4.18202	0.198527	-0.08478
C	-3.4689	1.315171	-0.07448
C	-2.08119	1.304944	-0.0646
H	-4.00722	2.254623	-0.0737
H	-1.48784	2.209401	-0.05578

$GaCl_3pyz$ (C_s)



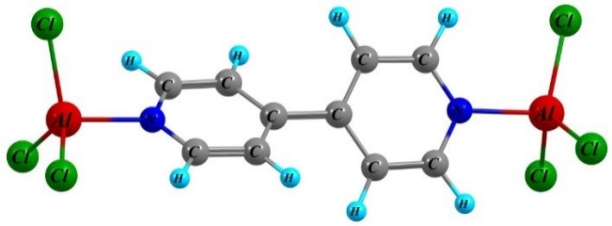
	X	Y	Z
Cl	1.10935	1.362208	1.823842
Cl	-2.11383	1.506919	0.000000
Cl	1.10935	1.362208	-1.823842
Ga	-0.00665	0.995097	0.000000
N	-0.06573	-1.07596	0.000000
C	1.095673	-1.73097	0.000000
C	1.10935	-3.11613	0.000000
H	2.000858	-1.13653	0.000000
H	2.047814	-3.65599	0.000000
N	-0.01033	-3.82945	0.000000
C	-1.15542	-3.16155	0.000000
C	-1.19905	-1.77455	0.000000
H	-2.07186	-3.73815	0.000000
H	-2.12449	-1.21299	0.000000

$GaBr_3pyz$ (C_1)



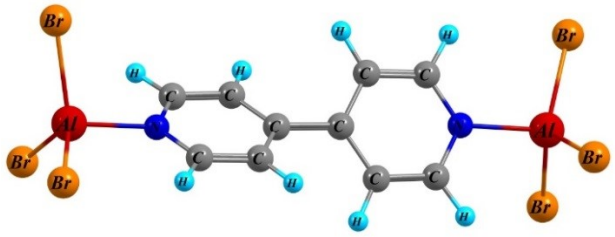
	X	Y	Z
Ga	0.544976	-0.00062	0.003753
Br	0.863529	-1.03233	2.062388
Br	1.208499	2.220936	-0.177691
Br	0.93026	-1.36792	-1.839126
N	-1.53163	0.130704	-0.039924
C	-2.19163	1.286717	-0.027068
C	-2.22778	-1.00701	-0.053039
H	-1.60073	2.193484	-0.017275
H	-1.66701	-1.9334	-0.067368
N	-4.28718	0.170649	-0.041586
C	-3.6124	-0.97265	-0.053076
C	-3.5795	1.291263	-0.028972
H	-4.18411	-1.89191	-0.063064
H	-4.12302	2.227752	-0.020096

$(AlCl_3)_2$(bipy) (C_2)



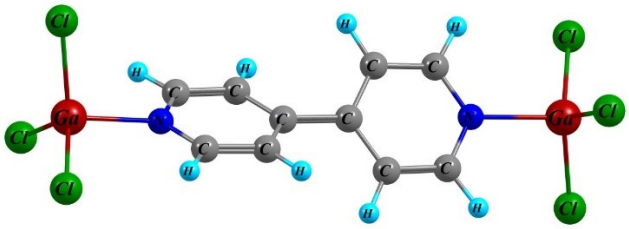
	X	Y	Z
Cl	-1.654028	5.894276	-1.217934
Cl	1.901584	6.058061	-0.750985
Cl	-0.317141	5.846932	2.061477
Cl	-1.901584	-6.058061	-0.750985
Cl	1.654028	-5.894276	-1.217934
Cl	0.317141	-5.846932	2.061477
Al	0.015892	5.490529	0.008462
Al	-0.015892	-5.490529	0.008462
N	0.074754	3.506323	-0.043108
N	-0.074754	-3.506323	-0.043108
C	-1.027287	2.854418	0.349904
C	1.146716	2.810870	-0.433297
C	1.154567	1.429462	-0.441295
C	-1.095037	1.477982	0.361514
C	0.015892	0.739580	-0.039886
C	-0.015892	-0.739580	-0.039886
C	-1.154567	-1.429462	-0.441295
C	1.095037	-1.477982	0.361514
C	-1.146716	-2.810870	-0.433297
C	1.027287	-2.854418	0.349904
H	-1.862887	3.469526	0.660709
H	2.003796	3.392984	-0.745254
H	2.036286	0.905323	-0.782846
H	-1.997714	0.991686	0.704040
H	-2.036286	-0.905323	-0.782846
H	1.997714	-0.991686	0.704040
H	-2.003796	-3.392984	-0.745254
H	1.862887	-3.469526	0.660709

$(AlBr_3)_2(bipy)$ (C_2)



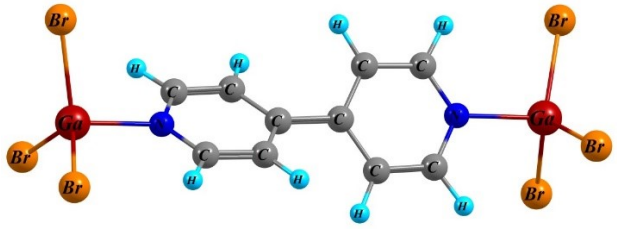
	X	Y	Z
Br	-1.700979	5.897518	-1.445238
Br	2.085910	6.152277	-0.701464
Br	-0.483654	5.908810	2.178552
Br	-2.085910	-6.152277	-0.701464
Br	1.700979	-5.897518	-1.445238
Br	0.483654	-5.908810	2.178552
Al	0.019888	5.494243	-0.005672
Al	-0.019888	-5.494243	-0.005672
N	0.092936	3.506767	-0.028502
N	-0.092936	-3.506767	-0.028502
C	-1.013270	2.859612	0.363275
C	1.161837	2.804967	-0.416383
C	1.162450	1.423453	-0.423079
C	-1.087770	1.484063	0.375846
C	0.019888	0.739408	-0.023385
C	-0.019888	-0.739408	-0.023385
C	-1.162450	-1.423453	-0.423079
C	1.087770	-1.484063	0.375846
C	-1.161837	-2.804967	-0.416383
C	1.013270	-2.859612	0.363275
H	-1.845656	3.479110	0.673678
H	2.023513	3.380861	-0.727415
H	2.042380	0.895270	-0.762991
H	-1.993678	1.003288	0.717554
H	-2.042380	-0.895270	-0.762991
H	1.993678	-1.003288	0.717554
H	-2.023513	-3.380861	-0.727415
H	1.845656	-3.479110	0.673678

$(GaCl_3)_2$(bipy) (C_2)



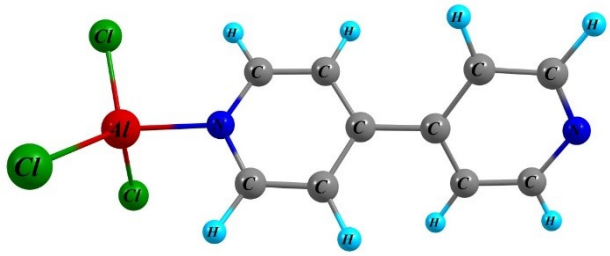
	X	Y	Z
Ga	-0.011207	5.567739	-0.013078
Ga	0.011207	-5.567739	-0.013078
Cl	2.090473	6.081903	-0.189525
Cl	-0.987663	5.995198	1.879151
Cl	-1.242327	5.905760	-1.766196
Cl	1.242327	-5.905760	-1.766196
Cl	-2.090473	-6.081903	-0.189525
Cl	0.987663	-5.995198	1.879151
N	0.054281	3.503278	0.043220
N	-0.054281	-3.503278	0.043220
C	-1.043979	2.848714	0.433044
C	-1.103995	1.470559	0.441058
C	0.011207	0.739790	0.039395
C	1.146977	1.436925	-0.360320
C	1.130710	2.818093	-0.349153
C	-1.130710	-2.818093	-0.349153
C	-1.146977	-1.436925	-0.360320
C	-0.011207	-0.739790	0.039395
C	1.103995	-1.470559	0.441058
C	1.043979	-2.848714	0.433044
H	-1.878661	3.460359	0.753061
H	-2.003666	0.977970	0.782730
H	2.031964	0.917815	-0.701277
H	1.986607	3.406990	-0.654115
H	-1.986607	-3.406990	-0.654115
H	-2.031964	-0.917815	-0.701277
H	2.003666	-0.977970	0.782730
H	1.878661	-3.460359	0.753061

$(GaBr_3)_2$(bipy) (C_2)



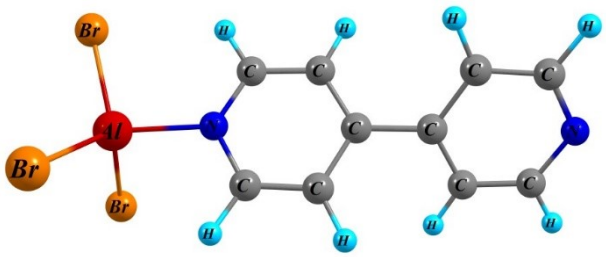
	X	Y	Z
Br	-2.119747	6.201618	0.684125
Br	1.750977	5.946888	1.509595
Br	0.572407	5.965834	-2.221548
Br	-1.750977	-5.946888	1.509595
Br	-0.572407	-5.965834	-2.221548
Br	2.119747	-6.201618	0.684125
Ga	0.014214	5.575381	0.004564
Ga	-0.014214	-5.575381	0.004564
N	-0.066710	3.503685	0.022021
N	0.066710	-3.503685	0.022021
C	-1.141037	2.814145	0.410062
C	1.034303	2.852597	-0.368012
C	-1.152407	1.432364	0.418354
C	1.099126	1.475424	-0.379700
C	-0.014214	0.739652	0.019405
C	0.014214	-0.739652	0.019405
C	-1.099126	-1.475424	-0.379700
C	1.152407	-1.432364	0.418354
C	-1.034303	-2.852597	-0.368012
C	1.141037	-2.814145	0.410062
H	-1.998626	3.398333	0.719424
H	1.870972	3.466548	-0.679114
H	-2.036103	0.910132	0.757956
H	2.001381	0.987046	-0.720575
H	-2.001381	-0.987046	-0.720575
H	2.036103	-0.910132	0.757956
H	-1.870972	-3.466548	-0.679114
H	1.998626	-3.398333	0.719424

$AlCl_3bipy$ (C_1)



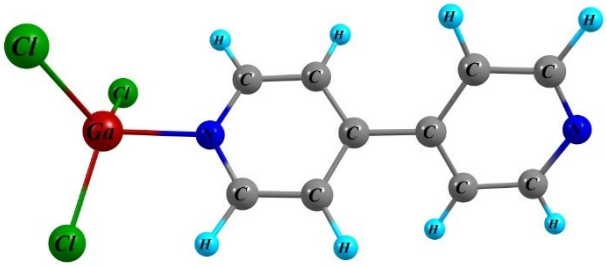
	X	Y	Z
Cl	-3.30857	-1.53057	-1.402953
Cl	-3.51406	1.949918	-0.567112
Cl	-3.33311	-0.55074	1.995612
Al	-2.91988	0.002615	-0.001682
N	-0.94789	0.085305	-0.014817
N	6.099443	-0.03154	0.004116
C	-0.28787	-1.02524	0.342591
C	-0.25336	1.172202	-0.368479
C	1.126537	1.185234	-0.374073
C	1.087642	-1.085	0.356885
C	1.827423	0.039767	-0.006830
C	3.305621	0.015342	-0.002822
C	4.005954	-1.11955	-0.398423
C	4.041663	1.126059	0.396511
C	5.392537	-1.08896	-0.380881
C	5.426497	1.048942	0.385703
H	-0.89828	-1.87427	0.625207
H	-0.83776	2.037056	-0.653512
H	1.64764	2.079443	-0.686354
H	1.577711	-1.99556	0.671973
H	3.48716	-2.00545	-0.741021
H	3.551367	2.028733	0.737249
H	5.96023	-1.95826	-0.693838
H	6.021247	1.898832	0.70166

$AlBr_3bipy$ (C_1)



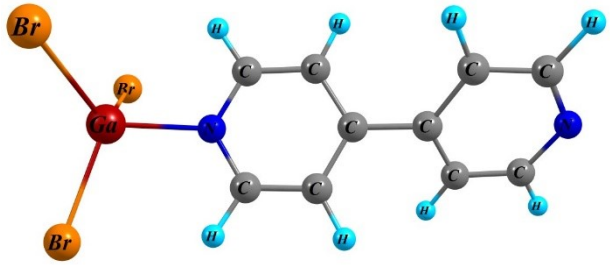
	X	Y	Z
Br	-2.36898	-1.68156	-1.484519
Br	-2.663	2.082611	-0.676313
Br	-2.4626	-0.5297	2.15633
Al	-1.97859	0.01267	-0.006058
N	-0.0043	0.106957	0.002702
N	7.043366	-0.00246	-0.013642
C	0.658248	-1.00464	0.355581
C	0.689596	1.198304	-0.339446
C	2.069331	1.213744	-0.343316
C	2.033502	-1.06183	0.369635
C	2.771995	0.065988	0.012069
C	4.249992	0.041934	0.006561
C	4.947134	-1.0867	-0.411737
C	4.988625	1.147511	0.415083
C	6.333811	-1.05493	-0.407152
C	6.373352	1.071684	0.390343
H	0.050392	-1.85755	0.632143
H	0.10497	2.064615	-0.619139
H	2.588556	2.111569	-0.648202
H	2.524766	-1.97416	0.677654
H	4.42559	-1.9678	-0.762507
H	4.500756	2.044888	0.772879
H	6.899279	-1.9189	-0.738432
H	6.97054	1.917406	0.712808

$GaCl_3bipy$ (C_1)



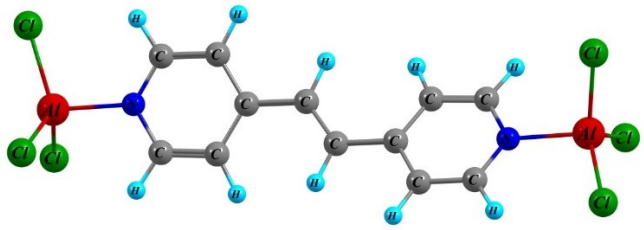
	X	Y	Z
Ga	-2.63955	0.001881	-0.005583
Cl	-3.18883	2.090199	-0.258050
Cl	-3.08512	-0.90256	1.920359
Cl	-3.00607	-1.29827	-1.707083
N	-0.59086	0.073241	0.036721
N	6.452694	-0.02884	-0.018528
C	0.069711	-1.03516	0.390351
C	1.44664	-1.09205	0.391946
C	2.180275	0.033265	0.018950
C	1.474319	1.177914	-0.342849
C	0.094538	1.161716	-0.324704
C	5.743595	-1.08826	-0.394069
C	4.356997	-1.12188	-0.395513
C	3.658678	0.011764	0.007078
C	4.396951	1.12445	0.396601
C	5.781752	1.050515	0.369657
H	-0.53771	-1.88269	0.684549
H	1.942063	-2.00071	0.704358
H	1.991465	2.072662	-0.660334
H	-0.4959	2.025835	-0.602116
H	6.309662	-1.95666	-0.712426
H	3.836175	-2.0092	-0.731328
H	3.908756	2.026542	0.74189
H	6.378226	1.902117	0.677586

$GaBr_3bipy$ (C_1)



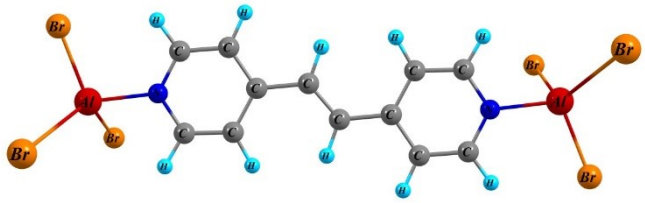
	X	Y	Z
Br	-2.50084	2.147349	-0.683367
Br	-2.23242	-1.71897	-1.520962
Br	-2.31411	-0.55501	2.20624
Ga	-1.85805	0.013223	-0.006034
N	0.19748	0.099302	-0.000340
N	7.241204	-0.00213	-0.010083
C	0.885827	1.194304	-0.333435
C	0.856051	-1.01453	0.341709
C	2.266032	1.211641	-0.337444
C	2.232463	-1.07108	0.355396
C	2.969136	0.060891	0.008551
C	4.447451	0.03878	0.004844
C	5.184072	1.140028	0.428216
C	5.146969	-1.08372	-0.425688
C	6.568955	1.066273	0.405241
C	6.533587	-1.05053	-0.417629
H	0.29847	2.06211	-0.605368
H	0.247164	-1.86963	0.610221
H	2.785432	2.112188	-0.634122
H	2.725413	-1.98539	0.654975
H	4.694367	2.032398	0.795888
H	4.627209	-1.96116	-0.788107
H	7.164455	1.908869	0.738934
H	7.10067	-1.909999	-0.757852

$(AlCl_3)_2$(bpe) (C_2)



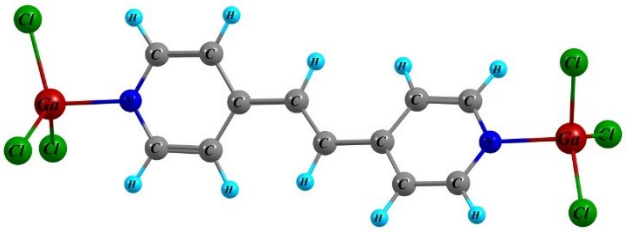
	X	Y	Z
Al	-0.052867	6.627066	-0.023569
Cl	-1.957732	7.330206	-0.604356
Cl	0.517520	7.011385	1.973520
Cl	1.508817	6.890345	-1.421603
N	-0.261505	4.660060	-0.015103
C	0.818046	3.932567	0.311037
H	1.716315	4.490976	0.544034
C	0.789496	2.558642	0.354918
H	1.683780	2.027661	0.646716
C	-0.395796	1.885636	0.047225
C	-1.508817	2.658352	-0.276001
H	-2.455135	2.192602	-0.514877
C	-1.406608	4.035185	-0.301702
H	-2.245603	4.670522	-0.553077
C	-0.514014	0.425079	0.057304
H	-1.529086	0.044443	0.024099
N	0.261505	-4.660060	-0.015103
C	-0.818046	-3.932567	0.311037
H	-1.716315	-4.490976	0.544034
C	-0.789496	-2.558642	0.354918
H	-1.683780	-2.027661	0.646716
C	0.395796	-1.885636	0.047225
C	1.508817	-2.658352	-0.276001
H	2.455135	-2.192602	-0.514877
C	1.406608	-4.035185	-0.301702
H	2.245603	-4.670522	-0.553077
C	0.514014	-0.425079	0.057304
H	1.529086	-0.044443	0.024099
Al	0.052867	-6.627066	-0.023569
Cl	1.957732	-7.330206	-0.604356
Cl	-0.517520	-7.011385	1.973520
Cl	-1.508817	-6.890345	-1.421603

$(AlBr_3)_2$(bpe) (C_2)



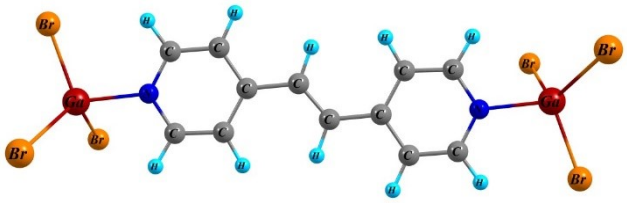
	X	Y	Z
Br	-1.97545	7.513598	0.000097
Br	1.336503	6.947015	-1.910206
Br	1.336259	6.946391	1.910529
Al	0.128423	6.638594	0.000038
N	-0.13921	4.675789	-0.000246
C	0.910252	2.539944	-0.000968
H	1.837166	1.98611	-0.001562
C	0.966249	3.912754	-0.000882
H	1.910737	4.442497	-0.001358
C	-0.33306	1.900858	-0.000354
C	-1.46745	2.70933	0.000282
H	-2.4571	2.273298	0.000750
C	-0.49698	0.445065	-0.000373
H	-1.52642	0.105118	-0.000304
C	-1.3365	4.084204	0.000327
H	-2.19512	4.74283	0.000808
N	0.139209	-4.67579	-0.000246
C	-0.91025	-2.53994	-0.000968
H	-1.83717	-1.98611	-0.001562
C	-0.96625	-3.91275	-0.000882
H	-1.91074	-4.4425	-0.001358
C	0.333059	-1.90086	-0.000354
C	1.467454	-2.70933	0.000282
H	2.457096	-2.273298	0.00075
C	0.496977	-0.44507	-0.000373
H	1.526419	-0.10512	-0.000304
C	1.336503	-4.0842	0.000327
H	2.195122	-4.74283	0.000808
Br	1.97545	-7.5136	0.000097
Br	-1.33626	-6.94639	1.910529
Br	-1.3365	-6.94702	-1.910206
Al	-0.12842	-6.63859	0.000038

$(GaCl_3)_2$(bpe) (C_2)



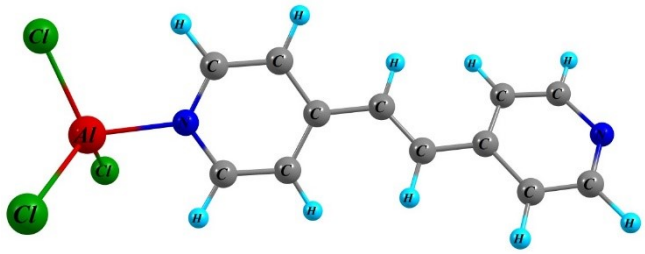
	X	Y	Z
Ga	-0.059688	6.703570	-0.020839
Cl	-2.049915	7.375145	-0.571300
Cl	0.578754	7.077330	2.021326
Cl	1.511287	6.959918	-1.498827
N	-0.262965	4.656783	-0.006073
C	0.818926	3.933555	0.311635
H	1.717978	4.492723	0.540828
C	0.791404	2.558607	0.353046
H	1.687481	2.027023	0.638323
C	-0.395471	1.886232	0.051131
C	-1.511287	2.658814	-0.264511
H	-2.458516	2.192324	-0.498575
C	-1.409638	4.036044	-0.287618
H	-2.250230	4.673152	-0.532046
C	-0.513659	0.425435	0.060014
H	-1.528956	0.045350	0.027432
N	0.262965	-4.656783	-0.006073
C	-0.818926	-3.933555	0.311635
H	-1.717978	-4.492723	0.540828
C	-0.791404	-2.558607	0.353046
H	-1.687481	-2.027023	0.638323
C	0.395471	-1.886232	0.051131
C	1.511287	-2.658814	-0.264511
H	2.458516	-2.192324	-0.498575
C	1.409638	-4.036044	-0.287618
H	2.250230	-4.673152	-0.532046
C	0.513659	-0.425435	0.060014
H	1.528956	-0.045350	0.027432
Ga	0.059688	-6.703570	-0.020839
Cl	2.049915	-7.375145	-0.571300
Cl	-0.578754	-7.077330	2.021326
Cl	-1.511287	-6.959918	-1.498827

$(GaBr_3)_2$(bpe) (C_2)



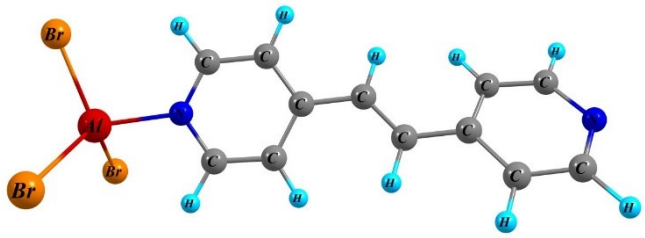
	X	Y	Z
Br	-2.06414	7.546128	0.000053
Br	1.344469	7.011771	-1.954694
Br	1.344341	7.011432	1.954866
Ga	0.111571	6.719455	0.000024
N	-0.14866	4.671818	-0.000161
C	0.905791	2.542084	-0.000841
H	1.833478	1.989409	-0.001458
C	0.958353	3.916186	-0.000795
H	1.901315	4.449327	-0.001329
C	-0.33619	1.900895	-0.000178
C	-1.47306	2.706465	0.000458
H	-2.46139	2.267255	0.000946
C	-0.49739	0.444465	-0.000173
H	-1.52635	0.102957	-0.000110
C	-1.34447	4.081961	0.000455
H	-2.20384	4.740625	0.000922
N	0.148663	-4.67182	-0.000161
C	-0.90579	-2.54208	-0.000841
H	-1.83348	-1.98941	-0.001458
C	-0.95835	-3.91619	-0.000795
H	-1.90132	-4.44933	-0.001329
C	0.336194	-1.9009	-0.000178
C	1.47306	-2.70647	0.000458
H	2.461385	-2.267255	0.000946
C	0.497392	-0.44447	-0.000173
H	1.526348	-0.10296	-0.00011
C	1.344469	-4.08196	0.000455
H	2.203837	-4.74063	0.000922
Br	2.064135	-7.54613	0.000053
Br	-1.34434	-7.01143	1.954866
Br	-1.34447	-7.01177	-1.954694
Ga	-0.11157	-6.71946	0.000024

$AlCl_3bpe$ (C_1)



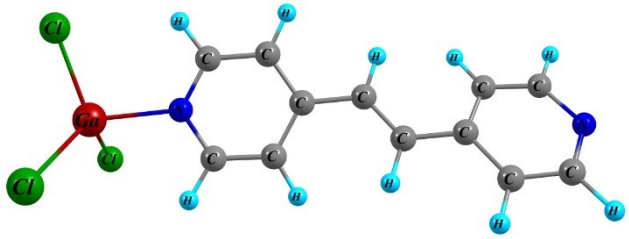
	X	Y	Z
Al	3.826299	-0.0926	-0.015059
Cl	4.61194	1.775646	-0.618425
Cl	4.212033	-0.65072	1.986605
Cl	4.053346	-1.68008	-1.393990
N	1.877617	0.187707	-0.013024
C	1.101476	-0.86788	0.282082
H	1.620027	-1.79516	0.493912
C	-0.26936	-0.78324	0.320039
H	-0.83785	-1.66272	0.584853
C	-0.89547	0.435726	0.040208
C	-0.0708	1.522677	-0.248784
H	-0.49596	2.493729	-0.463647
C	1.299173	1.364999	-0.270995
H	1.969276	2.183605	-0.498638
C	-2.34698	0.616467	0.043823
H	-2.68451	1.646734	0.014731
N	-7.4918	0.021509	-0.055041
C	-6.71723	1.059644	0.254069
H	-7.23039	1.988618	0.477209
C	-5.33517	1.001	0.30557
H	-4.77444	1.882904	0.584254
C	-4.69851	-0.20597	0.018714
C	-5.50885	-1.29464	-0.291841
H	-5.07206	-2.260094	-0.514907
C	-6.88624	-1.12997	-0.32002
H	-7.5303	-1.96704	-0.566292
C	-3.2422	-0.37385	0.033666
H	-2.89984	-1.40348	0.000334

$AlBr_3bpe$ (C_1)



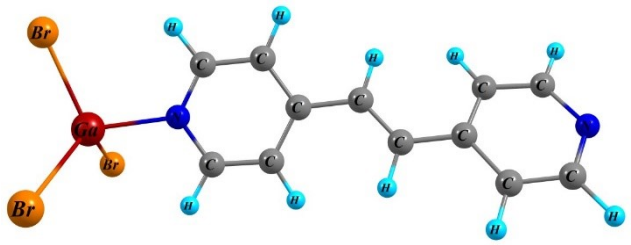
	X	Y	Z
Al	2.718731	-0.03228	-0.012605
Br	3.610164	1.971848	-0.641841
Br	3.156323	-0.67897	2.132057
Br	2.936928	-1.71643	-1.539504
N	0.769181	0.259652	0.017686
C	-0.00432	-0.80036	0.307754
H	0.51628	-1.72786	0.513253
C	-1.3748	-0.72007	0.348212
H	-1.93969	-1.60338	0.607782
C	-2.00574	0.498501	0.076934
C	-1.18452	1.590879	-0.200559
H	-1.61238	2.562816	-0.405826
C	0.185856	1.437931	-0.226684
H	0.851223	2.26227	-0.447840
C	-3.45794	0.671463	0.076262
H	-3.80163	1.699926	0.061415
N	-8.59745	0.037638	-0.077107
C	-7.83382	1.078957	0.24846
H	-8.35625	2.001588	0.476205
C	-6.45183	1.030835	0.310727
H	-5.9003	1.914652	0.601461
C	-5.80329	-0.16834	0.017546
C	-6.60222	-1.2603	-0.310477
H	-6.15593	-2.219941	-0.539633
C	-7.98067	-1.10626	-0.348363
H	-8.61569	-1.94615	-0.608154
C	-4.34596	-0.3249	0.042256
H	-3.99522	-1.35109	-0.006176

$GaCl_3bpe$ (C_1)



	X	Y	Z
Ga	3.484478	-0.07554	-0.009798
Cl	4.235802	1.860351	-0.654238
Cl	3.852459	-0.61264	2.063838
Cl	3.721808	-1.73225	-1.399002
N	1.457257	0.19002	-0.025801
C	0.685801	-0.87378	0.239452
H	1.205217	-1.80621	0.426099
C	-0.68603	-0.79109	0.276625
H	-1.25411	-1.67763	0.517565
C	-1.31211	0.434076	0.026236
C	-0.488	1.528687	-0.235867
H	-0.9143	2.503976	-0.428489
C	0.882554	1.37278	-0.257214
H	1.554639	2.196469	-0.463019
C	-2.76393	0.615089	0.033725
H	-3.10013	1.645943	0.011846
N	-7.91133	0.018267	-0.041695
C	-7.13531	1.062178	0.243652
H	-7.64743	1.994737	0.453922
C	-5.75295	1.005554	0.286172
H	-5.19177	1.893166	0.544792
C	-5.11703	-0.20571	0.015727
C	-5.92885	-1.29995	-0.270367
H	-5.49291	-2.268861	-0.479739
C	-7.30664	-1.13706	-0.291054
H	-7.95167	-1.97888	-0.518101
C	-3.66066	-0.37378	0.02352
H	-3.32007	-1.40384	-0.01249

$GaBr_3bpe$ (C_1)

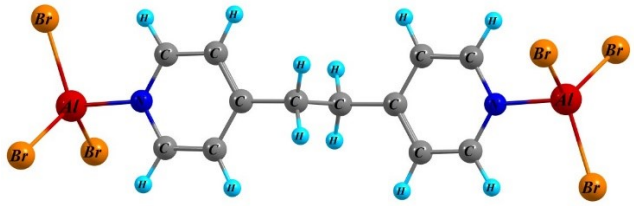


	X	Y	Z
Ga	2.550639	-0.03062	-0.012532
Br	3.404478	2.025352	-0.698353
Br	2.965402	-0.63374	2.200239
Br	2.763153	-1.79351	-1.526270
N	0.519104	0.25506	0.002061
C	-0.25093	-0.8091	0.272144
H	0.268905	-1.74115	0.459375
C	-1.62243	-0.72843	0.313265
H	-2.18826	-1.61556	0.557388
C	-2.25159	0.494928	0.062085
C	-1.4296	1.59129	-0.198335
H	-1.8573	2.56641	-0.388765
C	-0.05874	1.437329	-0.224356
H	0.609234	2.26422	-0.431300
C	-3.70413	0.669487	0.065476
H	-4.04615	1.698603	0.05828
N	-8.84657	0.035538	-0.064589
C	-8.08108	1.080589	0.244327
H	-8.60231	2.005536	0.465389
C	-6.6987	1.033813	0.297708
H	-6.14612	1.921395	0.574473
C	-6.05131	-0.16808	0.013165
C	-6.85215	-1.26363	-0.29791
H	-6.40694	-2.225532	-0.51964
C	-8.23091	-1.11088	-0.327711
H	-8.86724	-1.95383	-0.574145
C	-4.59388	-0.32513	0.030338
H	-4.24491	-1.35166	-0.022609

$(AlCl_3)_2$(bpa) (C_i)

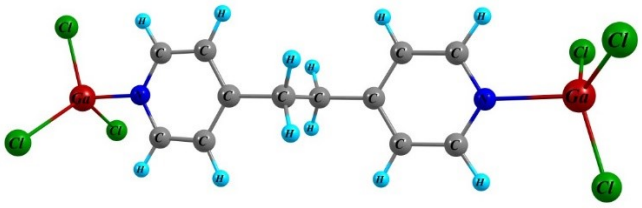
	X	Y	Z
Al	6.520456	0.035475	0.460413
Cl	7.115575	2.061628	0.403925
Cl	7.017595	-1.037543	2.210825
Cl	6.800169	-1.065548	-1.321450
N	4.549613	0.124887	0.575407
C	3.890857	-1.038569	0.669031
H	4.501832	-1.932635	0.694485
C	2.515935	-1.093586	0.733275
H	2.024859	-2.054368	0.814235
C	1.778587	0.087063	0.702175
C	2.477929	1.284329	0.607672
H	1.957121	2.232560	0.587505
C	3.857464	1.268292	0.546868
H	4.442580	2.175689	0.475709
C	0.278029	0.061719	0.716463
H	-0.107528	0.973615	1.175800
H	-0.075924	-0.780795	1.313484
N	-4.549613	-0.124887	-0.575407
C	-3.890857	1.038569	-0.669031
H	-4.501832	1.932635	-0.694485
C	-2.515935	1.093586	-0.733275
H	-2.024859	2.054368	-0.814235
C	-1.778587	-0.087063	-0.702175
C	-2.477929	-1.284329	-0.607672
H	-1.957121	-2.232560	-0.587505
C	-3.857464	-1.268292	-0.546868
H	-4.442580	-2.175689	-0.475709
C	-0.278029	-0.061719	-0.716463
H	0.107528	-0.973615	-1.175800
H	0.075924	0.780795	-1.313484
Al	-6.520456	-0.035475	-0.460413
Cl	-7.115575	-2.061628	-0.403925
Cl	-7.017595	1.037543	-2.210825
Cl	-6.800169	1.065548	1.321450

$(AlBr_3)_2$(bpa) (C_i)



	X	Y	Z
Al	6.521186	0.038810	0.459296
Br	7.207079	2.212353	0.397747
Br	7.076045	-1.124125	2.341283
Br	6.805821	-1.143862	-1.471698
N	4.548040	0.130525	0.585846
C	3.890618	-1.034448	0.681914
H	4.502376	-1.927912	0.710169
C	2.516089	-1.091942	0.744208
H	2.027626	-2.053908	0.826565
C	1.775687	0.086764	0.708375
C	2.472819	1.284975	0.612689
H	1.950635	2.232368	0.589202
C	3.852354	1.272121	0.553799
H	4.433654	2.181750	0.480413
C	0.275284	0.058520	0.717899
H	-0.113468	0.967462	1.180400
H	-0.079130	-0.787652	1.309379
N	-4.548040	-0.130525	-0.585846
C	-3.890618	1.034448	-0.681914
H	-4.502376	1.927912	-0.710169
C	-2.516089	1.091942	-0.744208
H	-2.027626	2.053908	-0.826565
C	-1.775687	-0.086764	-0.708375
C	-2.472819	-1.284975	-0.612689
H	-1.950635	-2.232368	-0.589202
C	-3.852354	-1.272121	-0.553799
H	-4.433654	-2.181750	-0.480413
C	-0.275284	-0.058520	-0.717899
H	0.113468	-0.967462	-1.180400
H	0.079130	0.787652	-1.309379
Al	-6.521186	-0.038810	-0.459296
Br	-7.207079	-2.212353	-0.397747
Br	-7.076045	1.124125	-2.341283
Br	-6.805821	1.143862	1.471698

$(GaCl_3)_2$(bpa) (C_i)

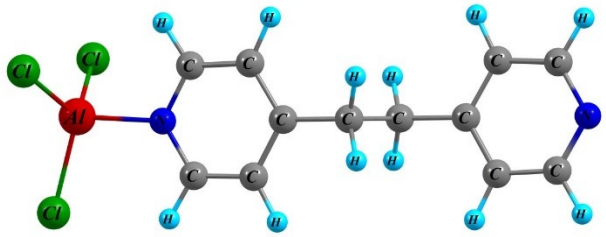


	X	Y	Z
Ga	-6.5706	-0.02648	0.725175
Cl	-7.07917	2.015222	1.265982
Cl	-7.39656	-0.79009	-1.132676
Cl	-6.52567	-1.4833	2.337121
N	-4.57444	0.111533	0.259292
C	-3.95813	-1.00524	-0.143919
H	-4.57284	-1.89483	-0.211537
C	-2.61592	-1.01992	-0.458277
H	-2.15523	-1.94268	-0.785655
C	-1.87439	0.153962	-0.357743
C	-2.53461	1.30415	0.059200
H	-2.00898	2.245976	0.146899
C	-3.88172	1.248747	0.358862
H	-4.43841	2.118179	0.684990
C	-0.39988	0.163888	-0.63843
H	-0.09648	1.143479	-1.012172
H	-0.16117	-0.56957	-1.41078
N	4.574438	-0.11153	-0.259292
C	3.958132	1.005244	0.143919
H	4.572838	1.89483	0.211537
C	2.615923	1.01992	0.458277
H	2.155226	1.942676	0.785655
C	1.874386	-0.15396	0.357743
C	2.534611	-1.304150	-0.0592
H	2.008984	-2.24598	-0.146899
C	3.881722	-1.24875	-0.358862
H	4.438408	-2.11818	-0.68499
C	0.399878	-0.16389	0.63843
H	0.096481	-1.14348	1.012172
H	0.161165	0.56957	1.41078
Ga	6.570603	0.02648	-0.725175
Cl	7.079165	-2.01522	-1.265982
Cl	7.396555	0.790092	1.132676
Cl	6.525671	1.483301	-2.337121

$(GaBr_3)_2(bpa)$ (C_i)

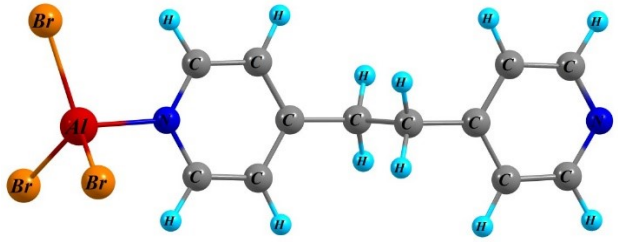
	X	Y	Z
Ga	6.600223	0.039404	0.457964
Br	7.247050	2.275364	0.425667
Br	7.133147	-1.176793	2.371997
Br	6.864575	-1.148856	-1.529697
N	4.544423	0.126573	0.590023
C	3.889727	-1.036022	0.692839
H	4.501301	-1.929661	0.729170
C	2.513892	-1.091333	0.753599
H	2.023015	-2.051614	0.842080
C	1.776094	0.088357	0.708698
C	2.474967	1.285388	0.605202
H	1.953465	2.233044	0.574403
C	3.854995	1.269251	0.548387
H	4.439737	2.177148	0.470095
C	0.275405	0.062794	0.717337
H	-0.112061	0.975380	1.173770
H	-0.080857	-0.778660	1.314460
N	-4.544423	-0.126573	-0.590023
C	-3.889727	1.036022	-0.692839
H	-4.501301	1.929661	-0.729170
C	-2.513892	1.091333	-0.753599
H	-2.023015	2.051614	-0.842080
C	-1.776094	-0.088357	-0.708698
C	-2.474967	-1.285388	-0.605202
H	-1.953465	-2.233044	-0.574403
C	-3.854995	-1.269251	-0.548387
H	-4.439737	-2.177148	-0.470095
C	-0.275405	-0.062794	-0.717337
H	0.112061	-0.975380	-1.173770
H	0.080857	0.778660	-1.314460
Ga	-6.600223	-0.039404	-0.457964
Br	-7.247050	-2.275364	-0.425667
Br	-7.133147	1.176793	-2.371997
Br	-6.864575	1.148856	1.529697

$AlCl_3bpa$ (C_1)



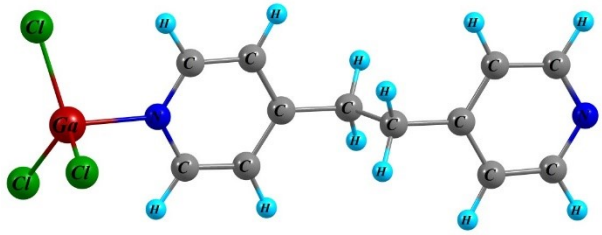
	X	Y	Z
Al	-3.81364	-0.00235	0.117779
Cl	-4.39343	2.016252	0.357857
Cl	-4.48636	-0.9529	-1.64606
Cl	-3.95943	-1.21687	1.842447
N	-1.86589	0.087132	-0.169035
C	-1.21916	-1.07475	-0.337088
H	-1.82753	-1.97047	-0.299208
C	0.140608	-1.1283	-0.550910
H	0.620856	-2.08838	-0.686624
C	0.877725	0.052235	-0.600559
C	0.189978	1.24796	-0.422379
H	0.710694	2.196132	-0.455213
C	-1.17348	1.231103	-0.210117
H	-1.74637	2.138457	-0.069681
C	2.365068	0.033992	-0.787493
H	2.679846	0.913053	-1.353404
H	2.659513	-0.84725	-1.360272
N	7.350245	-0.03377	-0.063647
C	6.671961	1.10817	-0.009689
H	7.250075	2.016513	-0.142645
C	5.303491	1.178233	0.20697
H	4.808864	2.141646	0.248477
C	4.583952	0.002284	0.380217
C	5.290661	-1.192025	0.323487
H	4.786794	-2.14168	0.458586
C	6.660505	-1.15722	0.102688
H	7.229636	-2.07983	0.061622
C	3.093013	0.021449	0.570165
H	2.775967	-0.85464	1.139928
H	2.79922	0.904448	1.142177

$AlBr_3bpa$ (C_1)



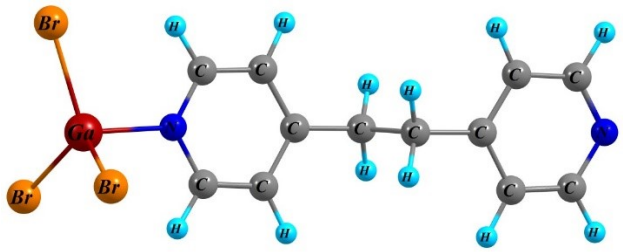
	X	Y	Z
Al	-2.72023	0.014225	0.054431
Br	-3.42883	2.182774	0.006651
Br	-3.41944	-1.28838	-1.684752
Br	-2.86039	-1.01919	2.085185
N	-0.77093	0.103882	-0.239789
C	-0.106	-1.06102	-0.271480
H	-0.7016	-1.95545	-0.132611
C	1.254402	-1.11835	-0.473651
H	1.74872	-2.0807	-0.498733
C	1.976287	0.05965	-0.653569
C	1.27153	1.257135	-0.614318
H	1.777733	2.203515	-0.751713
C	-0.09337	1.244768	-0.408410
H	-0.67853	2.154339	-0.377922
C	3.46461	0.037053	-0.830865
H	3.786302	0.911749	-1.399014
H	3.759493	-0.84861	-1.39718
N	8.445074	0.0005	-0.074422
C	7.775083	1.137088	0.083379
H	8.36145	2.048872	0.043301
C	6.404861	1.197895	0.295327
H	5.917683	2.157166	0.424291
C	5.675688	0.016991	0.351386
C	6.37433	-1.172627	0.186648
H	5.861683	-2.12656	0.2278
C	7.745412	-1.12855	-0.020959
H	8.307621	-2.04773	-0.146892
C	4.18347	0.026889	0.531746
H	3.867958	-0.85268	1.09743
H	3.880776	0.906557	1.103763

$GaCl_3bpa$ (C_1)



	X	Y	Z
Ga	-3.46929	-0.00218	0.108095
Cl	-4.09922	2.01056	-0.422507
Cl	-4.12999	-1.60996	-1.200902
Cl	-3.53829	-0.48111	2.225859
N	-1.45686	0.044115	-0.265913
C	-0.79989	-1.11247	-0.406926
H	-1.40271	-2.01184	-0.375830
C	0.565112	-1.15353	-0.598134
H	1.057607	-2.10988	-0.715962
C	1.290184	0.033518	-0.650824
C	0.587709	1.224893	-0.497845
H	1.099377	2.177871	-0.535211
C	-0.7787	1.195487	-0.308021
H	-1.3652	2.099031	-0.195439
C	2.780411	0.027203	-0.816221
H	3.097598	0.911386	-1.372639
H	3.088849	-0.84882	-1.389791
N	7.754663	-0.02167	-0.028151
C	7.072755	1.117355	0.039097
H	7.650269	2.029439	-0.068307
C	5.701336	1.18008	0.239331
H	5.203801	2.141394	0.292728
C	4.982763	-0.00058	0.381233
C	5.693416	-1.191930	0.31096
H	5.190327	-2.14519	0.42194
C	7.065752	-1.14977	0.108036
H	7.637669	-2.07016	0.056729
C	3.489328	0.010835	0.551286
H	3.168611	-0.86998	1.111721
H	3.183626	0.889233	1.124085

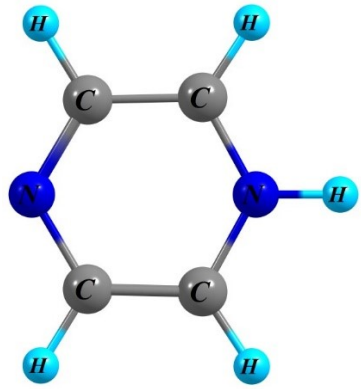
$GaBr_3bpa$ (C_1)



	X	Y	Z
Ga	-2.55262	0.013439	0.054165
Br	-3.2404	2.236746	-0.045126
Br	-3.25337	-1.36913	-1.68771
Br	-2.63006	-1.00039	2.153854
N	-0.52758	0.101603	-0.273626
C	0.137938	-1.06005	-0.291012
H	-0.45535	-1.95457	-0.140942
C	1.499771	-1.11341	-0.491047
H	1.999633	-2.07323	-0.504261
C	2.21587	0.066344	-0.681323
C	1.505683	1.261315	-0.657988
H	2.008462	2.208212	-0.804501
C	0.139854	1.243905	-0.454284
H	-0.45177	2.150403	-0.434506
C	3.705495	0.047484	-0.851095
H	4.029661	0.927121	-1.410089
H	4.004192	-0.83305	-1.423522
N	8.682363	-0.00292	-0.062345
C	8.015153	1.132579	0.113659
H	8.604962	2.042805	0.095613
C	6.643648	1.194049	0.317389
H	6.15873	2.152203	0.461983
C	5.910044	0.014917	0.344528
C	6.605907	-1.173691	0.160895
H	6.089538	-2.12632	0.179146
C	7.97843	-1.1304	-0.036442
H	8.538342	-2.04882	-0.177358
C	4.416721	0.025625	0.515213
H	4.096726	-0.85808	1.071944
H	4.111538	0.900891	1.092597

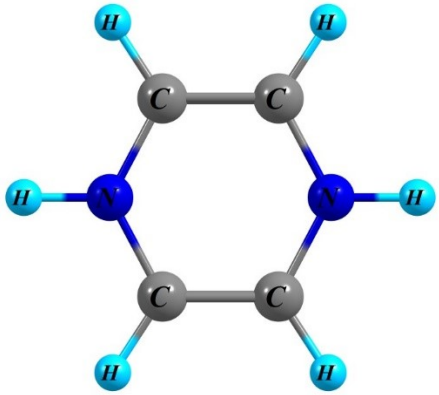
Fig. S31. Optimized structures and xyz coordinates for protonated ligands. M06-2X/def2-TZVPPD level of theory.

pyzH$^+$



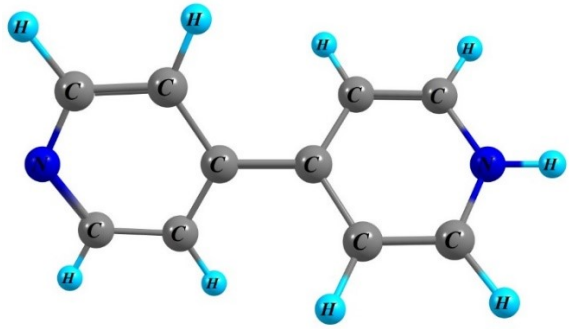
	X	Y	Z
N	0.000000	0.000000	-1.284324
N	0.000000	0.000000	1.417441
C	0.000000	1.172597	-0.641748
C	0.000000	-1.172597	-0.641748
C	0.000000	-1.142986	0.743381
C	0.000000	1.142986	0.743381
H	0.000000	2.074909	-1.234687
H	0.000000	-2.074909	-1.234687
H	0.000000	-2.064975	1.309485
H	0.000000	2.064975	1.309485
H	0.000000	0.000000	-2.301017

pyzH$_2^{2+}$



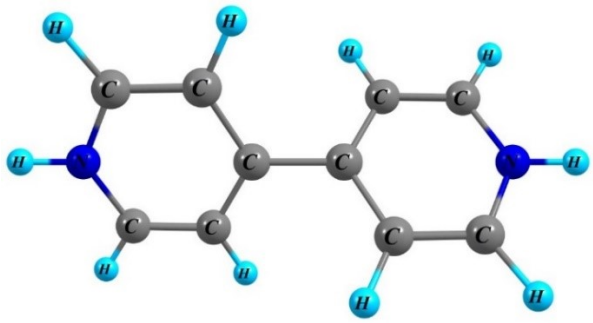
	X	Y	Z
N	0.000000	0.000000	1.321152
N	0.000000	0.000000	-1.321152
C	0.000000	1.181111	0.694034
C	0.000000	-1.181111	0.694034
C	0.000000	-1.181111	-0.694034
C	0.000000	1.181111	-0.694034
H	0.000000	2.088802	1.286544
H	0.000000	-2.088802	1.286544
H	0.000000	-2.088802	-1.286544
H	0.000000	2.088802	-1.286544
H	0.000000	0.000000	2.348195
H	0.000000	0.000000	-2.348195

bipyH$^+$



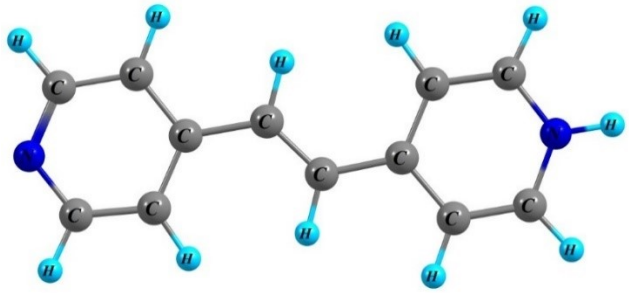
	X	Y	Z
C	0.000000	0.000000	0.786647
C	0.000000	0.000000	-0.684439
N	0.000000	0.000000	-3.423026
C	0.001164	1.201052	-1.406663
C	-0.001164	-1.201052	-1.406663
C	0.000000	-1.178366	-2.777060
C	0.000000	1.178366	-2.777060
H	-0.022125	2.153369	-0.898144
H	0.022125	-2.153369	-0.898144
H	0.008430	-2.067896	-3.389122
H	-0.008430	2.067896	-3.389122
N	0.000000	0.000000	3.569171
C	-0.662830	-0.995396	1.499983
C	0.662830	0.995396	1.499983
C	0.639283	0.942935	2.886498
C	-0.639283	-0.942935	2.886498
H	-1.219198	-1.776922	1.000632
H	1.219198	1.776922	1.000632
H	1.159300	1.692623	3.469946
H	-1.159300	-1.692623	3.469946
H	0.000000	0.000000	-4.435995

bipyH$_2^{2+}$



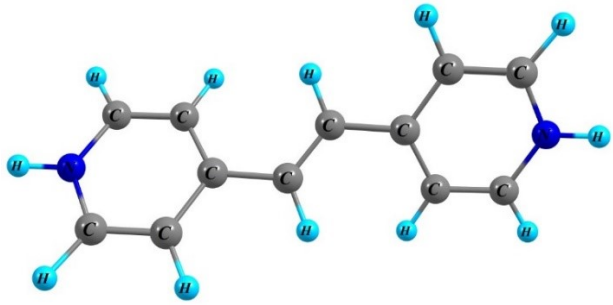
	X	Y	Z
C	0.000000	0.000000	0.743932
C	0.000000	0.000000	-0.743932
N	0.000000	0.000000	-3.464756
C	-0.437439	1.121358	-1.450364
C	0.437439	-1.121358	-1.450364
C	0.432837	-1.097384	-2.827408
C	-0.432837	1.097384	-2.827408
H	-0.804156	2.004219	-0.945943
H	0.804156	-2.004219	-0.945943
H	0.765547	-1.923033	-3.440524
H	-0.765547	1.923033	-3.440524
N	0.000000	0.000000	3.464756
C	-0.437439	-1.121358	1.450364
C	0.437439	1.121358	1.450364
C	0.432837	1.097384	2.827408
C	-0.432837	-1.097384	2.827408
H	-0.804156	-2.004219	0.945943
H	0.804156	2.004219	0.945943
H	0.765547	1.923033	3.440524
H	-0.765547	-1.923033	3.440524
H	0.000000	0.000000	4.482003
H	0.000000	0.000000	-4.482003

bpeH$^+$



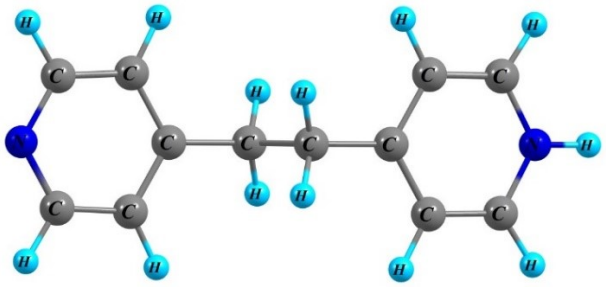
	X	Y	Z
C	0.000000	0.663403	0.000000
C	-1.254457	1.382095	0.000000
N	-3.579403	2.860039	0.000000
C	-2.519610	0.760777	0.000000
C	-1.234027	2.790221	0.000000
C	-2.399208	3.505399	0.000000
C	-3.657986	1.514682	0.000000
H	-2.622220	-0.312935	0.000000
H	-0.294046	3.322543	0.000000
H	-2.435557	4.584536	0.000000
H	-4.650403	1.089483	0.000000
C	0.115763	-0.675071	0.000000
H	0.888978	1.280808	0.000000
C	1.360995	-1.432799	0.000000
H	-0.779474	-1.287898	0.000000
N	3.679480	-2.988494	0.000000
C	2.625411	-0.840416	0.000000
C	1.297850	-2.824883	0.000000
C	2.479488	-3.553926	0.000000
C	3.741973	-1.658097	0.000000
H	2.755081	0.232379	0.000000
H	0.344113	-3.336124	0.000000
H	2.455464	-4.636755	0.000000
H	4.734931	-1.225699	0.000000
H	-4.434568	3.400544	0.000000
C	0.000000	0.663403	0.000000

bpeH$_2^{2+}$



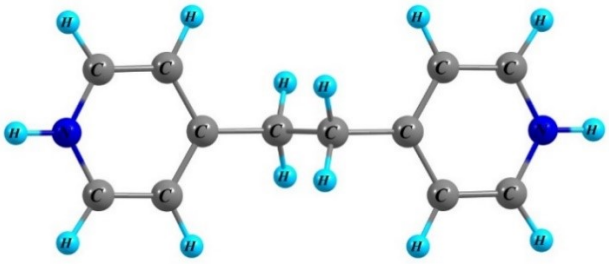
	X	Y	Z
C	-0.401398	0.533758	0.039863
C	-1.868986	0.474299	0.024442
N	-4.602135	0.454546	-0.041422
C	-2.587395	-0.665501	0.406426
C	-2.587395	1.607052	-0.374625
C	-3.961177	1.575037	-0.405500
C	-3.959483	-0.653391	0.363297
H	-2.093801	-1.557879	0.760962
H	-2.080340	2.515065	-0.668421
H	-4.572105	2.412694	-0.709455
H	-4.572553	-1.496212	0.647604
C	0.401398	-0.533758	0.039863
H	0.017817	1.532672	0.000556
C	1.868986	-0.474299	0.024442
H	-0.017817	-1.532672	0.000556
N	4.602135	-0.454546	-0.041422
C	2.587395	0.665501	0.406426
C	2.587395	-1.607052	-0.374625
C	3.961177	-1.575037	-0.405500
C	3.959483	0.653391	0.363297
H	2.093801	1.557879	0.760962
H	2.080340	-2.515065	-0.668421
H	4.572105	-2.412694	-0.709455
H	4.572553	1.496212	0.647604
H	-5.617288	0.445801	-0.064717
H	5.617288	-0.445801	-0.064717
C	-0.401398	0.533758	0.039863

bpaH$^+$



	X	Y	Z
C	0.276393	2.517013	1.199451
C	0.276393	2.517013	-1.199451
C	0.423135	1.811859	0.000000
C	0.004770	3.861118	1.179004
N	-0.122455	4.493167	0.000000
C	0.004770	3.861118	-1.179004
C	0.669706	0.339931	0.000000
H	1.244462	0.056071	-0.881845
H	1.244462	0.056071	0.881845
H	0.382670	2.014985	-2.150810
H	-0.113710	4.463312	-2.067492
H	-0.113710	4.463312	2.067492
H	0.382670	2.014985	2.150810
C	-0.670609	-0.432765	0.000000
C	-0.417578	-1.916108	0.000000
H	-1.249756	-0.148592	0.880636
H	-1.249756	-0.148592	-0.880636
C	-0.273951	-2.618521	-1.188803
C	-0.273951	-2.618521	1.188803
C	0.004770	-3.977774	-1.136009
H	-0.386909	-2.125596	-2.146527
C	0.004770	-3.977774	1.136009
H	-0.386909	-2.125596	2.146527
N	0.145546	-4.651718	0.000000
H	0.115978	-4.548423	-2.050388
H	0.115978	-4.548423	2.050388
H	-0.318815	5.486815	0.000000
C	0.276393	2.517013	1.199451

$bpaH_2^{2+}$



	X	Y	Z
C	0.152261	2.595853	1.198988
C	0.152261	2.595853	-1.198988
C	0.314412	1.898869	0.000000
C	-0.152261	3.936462	1.178587
N	-0.294225	4.562039	0.000000
C	-0.152261	3.936462	-1.178587
C	0.642815	0.430327	0.000000
H	1.241460	0.192263	-0.880041
H	1.241460	0.192263	0.880041
H	0.277963	2.104923	-2.153938
H	-0.281607	4.535782	-2.068166
H	-0.281607	4.535782	2.068166
H	0.277963	2.104923	2.153938
C	-0.152261	-2.595853	-1.198988
C	-0.152261	-2.595853	1.198988
C	-0.314412	-1.898869	0.000000
C	0.152261	-3.936462	-1.178587
N	0.294225	-4.562039	0.000000
C	0.152261	-3.936462	1.178587
C	-0.642815	-0.430327	0.000000
H	-1.241460	-0.192263	0.880041
H	-1.241460	-0.192263	-0.880041
H	-0.277963	-2.104923	2.153938
H	0.281607	-4.535782	2.068166
H	0.281607	-4.535782	-2.068166
H	-0.277963	-2.104923	-2.153938
H	-0.511908	5.553742	0.000000
H	0.511908	-5.553742	0.000000
C	0.152261	2.595853	1.198988