Supplementary information

For the manuscript "Versatile structures of group 13 metal halide complexes with 4,4′-bipy: from 1D coordination polymers to 2D and 3D metal-organic frameworks" by Tatiana N. Sevastianova et al.

Synthetic procedures.

$AlCl_3$bipy **(1)**: Synthesis 1: $AlCl_3$ (126.0 mg, 0.945 mmol) was sublimed at 80-90 ºC to bipy (151.8 mg, 0.972 mmol). The initial $AlCl_3$ to bipy ratio was 1:1.03. The system was stored at 160 ºC for several days, excess component was not removed. Single crystals suitable for the X-ray analysis have been grown by slow sublimation of the complexes in vacuum at circa 190-200 ºC during several weeks. Synthesis 2: bipy (279.6 mg, 1.7902 mmol) was sublimed at 80ºC to $AlCl_3$ (204.6 mg, 1.5344 mmol). The initial $AlCl_3$ to bipy ratio was 1:1.17. The system was stored at 120-160 ºC for several days. After that, an excess of bipy was sublimed (150-170 ºC, several days) into a special compartment, and sealed off. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 220-230 ºC during several weeks. IR (KBr pellet): 429m, 489vs, 533m, 583m, 649vs, 812s, 816s, 821s, 1019m, 1075m, 1222m, 1422s, 1490m, 1535m, 1619vs. Calculated: C 41.48; H 2.79; N 9.68). Found: C 41.72 ± 0.24; H 2.98 ± 0.19; N 9.61 ± 0.07.

$AlBr_3$bipy **(2)**: bipy (173.2 mg, 1.1089 mmol) was sublimed at 80ºC to $AlBr_3$ (206.0 mg, 0.7724 mmol). The$AlBr_3$ to bipy ratio was 1:1.44. The system was stored at 150-160 ºC for several days. After that, an excess of bipy was sublimed (80-90 ºC, 5 hours) into a special compartment, and sealed off, the mass was determined (53 mg, 0.3407mmol). The $AlBr_3$ to bipy ratio is 1.01:1, in agreement with the desired 1:1 complex composition. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 554m, 563m, 547m, 648s, 665s, 789w, 829m, 839w, 853w, 1018s, 1078s, 1223m, 1420s, 1491m, 1593m, 1616vs.

$GaCl_3$bipy **(3)**: bipy **(**95.7 mg, 0.613 mmol) bipy was sublimed at 80 ºC to $GaCl_3$ (69.4 mg, 0.394 mmol). The $GaCl_3$ to bipy ratio was 1:1.55. The system was stored at 150-160 ºC for several days. After that, an excess of bipy was sublimed (80-90 ºC, 5 hours) into a special compartment, and sealed off, the mass was determined (35.7mg, 0.229 mmol). The $GaCl_3$ to bipy ratio is 1:0.98, in agreement with the desired 1:1 complex composition. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 569m, 635vs, 729w, 789s, 812vs, 1011s, 1070vs, 1196w, 1219vs, 1360m, 1414vs, 1472m, 1483s, 1535s, 1595s, 1611s, 1632s.

$GaBr_3$bipy **(4)**: bipy (214.6 mg, 1.5789 mmol) was sublimed at 80ºC to $GaBr_3$ (461.2 mg, 1.4904 mmol). The $GaBr_3$ to bipy ratio was 1:1.06. The system was stored at 150-160 ºC for several days. Single crystals, suitable for X-ray structural analysis, were grown from the sample by sublimation at 190-200 ºC during several weeks.

$GaCl_3bipy_2$ **(5)**: $GaCl_3$ (0.1195 mg, 0.6787 mmol) was sublimed at 70 ºC to bipy (226.3 mg, 1.449 mmol). The $GaCl_3$ to bipy ratio was 1:2.14. The system was stored at 150-160 ºC for several days. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 478w, 488vw, 608m, 642s, 727vw, 737vw, 814vs, 856vw, 988vw, 1013m, 1067s, 1219m, 1408s, 1422sh, 1585m, 1616vs.

$(AlCl_3)_2$bipy **(6)**: bipy (124.4 mg, 0.797 mmol) was sublimed at 120 ºC to $AlCl_3$ (226.7 mg, 1.700 mmol). The $AlCl_3$ to bipy ratio was 2.13:1. The system was stored at 160 ºC for several days. After that, an excess of $AlCl_3$ was quantitatively sublimed (80-90 ºC, one day) into a special compartment and sealed off. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks.

$(GaCl_3)_2$bipy **(7)**: bipy (115.5 mg, 0.7395 mmol) was sublimed at 80 ºC to $GaCl_3$ (206.5 mg, 1.4794 mmol). The $GaCl_3$ to bipy ratio was 2.00:1. The system was stored at 150-160 ºC for several days. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 528m, 567m, 664s, 725w, 775m, 820vs, 1024s, 1080vs, 1223s, 1427vs, 1493m, 1535m, 1620vs.

$(AlBr_3)_2$bipy **(9)**: bipy (55.6 mg, 0.356 mmol) was sublimed at 80 ºC to $AlBr_3$ (192.1 mg, 0.7203 mmol). The $AlBr_3$ to bipy ratio was 2.02:1. The system was stored at 160 ºC for several days. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 436m, 444m, 453m, 492w, 500w, 563m, 662m, 783vs, 816vs, 1020m, 1080vs, 1198m, 1223s, 1233sh, 1423m, 1481m, 1614vs.

$(GaBr_3)_2$bipy **(10)**: bipy (81.7 mg, 0.5231 mmol) was sublimed at 80ºC to $GaBr_3$ (338.3 mg, 1.0932 mmol). The $GaBr_3$ to bipy ratio was 2.09:1. The system was stored at 150-160 ºC for several days. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 190-200 ºC during several weeks. IR (KBr pellet): 656m, 719w, 814s, 1020m, 1076s, 1221m, 1425s, 1493m, 1618vs.

$AlGaBr_6$bipy (**11**): $AlBr_3$ (152.9 mg, 0.5733 mmol) was sublimed at 80ºC to bipy (84.3 mg, 0.5398 mmol). Mixture was heated up till melting. Then $GaBr_3$ (173.3 mg, 0.5600 mmol) was sublimed at 80ºC to mixture of $AlBr_3$ with bipy. The $AlBr_3$ to bipy to $GaBr_3$ ratio was 1.06:1:1.04. The system was stored at 110 ºC for four days. Single crystals, suitable for X-ray structural analysis, were grown by sublimation at 220-230 ºC during several weeks.

Structural studies.

Crystals of **1-11** were taken from an ampule inside a glovebox filled with argon and covered with perfluorinated Fomblin® oil. The single crystal was taken to the pre-centered goniometer head with CryoMount® and directly attached to the diffractometer into a stream of cold nitrogen. The data were collected on an Agilent Technologies Gemini R Ultra diffractometer equipped with Ruby CCD detector and an Enhanced Ultra CuK_α sealed tube (λ = 1.54178 Å) and fine-focus MoK_α (λ = 0.71073 Å) sealed tube. The data for **1-6** and **8-11** were collected using CuK_α radiation and 1° ω scans or using MoK_α radiation and 0.5° ω scans for **7**. The *CrysAlis* software was used for data processing and absorption correction [*2*]. Using *Olex2* [*3*] the structures of **2-9** were solved by direct methods with *SIR-97* [*4*] and refined by full-matrix least-squares method against F^2 in anisotropic approximation using *SHELXL14*. All non-hydrogen atoms were refined anisotropically, while the hydrogen atoms were refined riding on pivot atoms. For the investigation of twinning and for structure checking the *PLATON* software was employed [*5*].

1 is racemically twinned with 0.40(2) ratio and contains disordered anions. Therefore, distance and displacement parameter restraints were used for refinement. **2** shows orthorhombic body centered pseudo symmetry which cannot be found in the model. All investigated crystals of **9** were non-merohedrally twinned. One with a very minor twin component was finally processed resulting in slightly increased quality factors. For the same reason the weak separated reflections below 0.87 Å were cut. Details of the diffraction experiments and refinements are given in Table S1.

The CIF files with comprehensive information on the details of the diffraction experiments and full tables of bond lengths and angles for **1-11** are deposited in Cambridge Crystallographic Data Centre under the deposition codes CCDC-1026689- CCDC-1026699, respectively.

Table S1. Crystal Structure Information for **1-11**.

Compound	**1** $AlCl_3$bipy	**2** $AlBr_3$bipy	**3** $GaCl_3$bipy	**4** $GaBr_3$bipy	**5** $GaCl_3$ 2bipy	**6** Al_2Cl_6bipy
Formula	$C_{20}H_{16}Al_2Cl_6N_4$	$C_{20}H_{16}Al_2Br_6N_4$	$C_{10}H_8Cl_3GaN_2$	$C_{20}H_{16}Br_6Ga_2N_4$	$C_{40}H_{32}Cl_6Ga_2N_8$	$C_{10}H_8N_2Al_2Cl_6$
$D_{calc.}$/ g cm^{-3}	1.429	2.109	1.785	2.297	1.554	1.627
μ/mm^{-1}	6.594	11.672	8.786	13.025	5.443	9.993
Formula Weight	579.03	845.79	332.25	931.27	976.87	422.84
Colour	colourless	colourless	colourless	colourless	colourless	colourless
Shape	prism	block	block	block	block	block
Max Size/mm	0.44	0.63	0.30	0.08	0.32	0.22
Mid Size/mm	0.32	0.38	0.21	0.06	0.20	0.17
Min Size/mm	0.16	0.10	0.18	0.05	0.15	0.12
T/K	123(2)	123.00(14)	123.0(2)	123(2)	123(2)	123(2)
Crystal System	orthorhombic	monoclinic	orthorhombic	monoclinic	orthorhombic	orthorhombic
Space Group	*Fdd*2	*I*2/*a*	*Pbcn*	*C*2/*c*	*Pnna*	*Pbca*
a/Å	7.08090(10)	13.20393(12)	13.5618(4)	22.3192(2)	16.34720(10)	15.5509(2)
b/Å	38.7664(4)	22.3430(2)	19.8375(7)	22.5024(2)	15.88050(10)	11.95200(10)
c/Å	39.2286(4)	18.06090(16)	9.1922(3)	13.22420(10)	16.08530(10)	18.5778(3)
α/°	90	90	90	90	90	90
β/°	90	90.1528(8)	90	125.8230(10)	90	90
γ/°	90	90	90	90	90	90
V/Å^3	10768.3(2)	5328.24(9)	2473.00(14)	5385.25(10)	4175.77(4)	3452.95(8)
Z	16	8	8	8	4	8
Z'	1	1	1	1	0.5	1
Θ_{min}/°	4.508	3.146	3.948	3.134	3.855	4.760
Θ_{max}/°	67.093	66.662	66.625	62.181	66.578	66.512
Measured Refl.	53286	32961	21045	10148	27755	15564
Independent Refl.	4817	4706	2183	4164	3689	3018
Reflections Used	4802	4631	2135	3003	3369	2630
R_{int}	0.0825	0.0423	0.0497	0.0310	0.0256	0.0529
Parameters	312	294	146	294	275	181
Restraints	65	0	0	0	0	0
Largest Peak	1.228	0.695	0.473	1.076	0.241	0.463
Deepest Hole	-1.048	-1.265	-0.425	-0.511	-0.453	-0.365
GooF	1.098	1.160	1.117	0.901	1.045	1.084
wR_2 (all data)	0.1817	0.0653	0.0772	0.0735	0.0734	0.0805
wR_2	0.1815	0.0649	0.0764	0.0713	0.0713	0.0744
R_1 (all data)	0.0677	0.0266	0.0296	0.0470	0.0281	0.0358
R_1	0.0675	0.0260	0.0288	0.0321	0.0258	0.0303
Flack Parameter	0.00(16)*	-	-	-	-	-

* Determined with SHELXL97 [1].

Compound	**7** Ga_2Cl_6bipy	**8** $AlCl_3bipyGaCl_3$	**9** Al_2Br_6bipy	**10** Ga_2Br_6bipy	**11** $AlBr_3bipyGaBr_3$
Formula	$C_{10}H_8N_2Cl_6Ga_2$	$C_{10}H_8Al_{1.1}Cl_6Ga_{0.9}N_2$	$C_{10}H_8Al_2Br_6N_2$	$C_{10}H_8Br_6Ga_2N_2$	$C_{10}H_8Al_{1.1}Br_6Ga_{0.9}N_2$
$D_{calc.}$/ g cm^{-3}	1.945	1.765	2.338	2.662	2.503
μ/mm^{-1}	4.016	2.401	15.617	17.874	16.763
Formula Weight	508.32	461.31	689.60	775.08	728.07
Colour	colourless	colourless	colourless	colourless	colourless
Shape	block	block	rod	rod	block
Max Size/mm	0.49	0.08	0.19	0.61	0.08
Mid Size/mm	0.37	0.05	0.08	0.16	0.05
Min Size/mm	0.28	0.03	0.07	0.06	0.04
T/K	123.05(10)	123(2)	192.9(2)	123(2)	123.15
Crystal System	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic
Space Group	*Pbca*	*Pbca*	$P2_1/c$	$P2_1/c$	$P2_1/c$
a/Å	15.5909(7)	15.581(5)	9.8192(4)	9.79360(10)	9.7971(2)
b/Å	11.9714(6)	11.971(5)	16.4152(5)	16.3623(2)	16.3329(3)
c/Å	18.6015(8)	18.613(5)	12.4071(4)	12.3274(2)	12.3295(3)
α/°	90	90	90	90	90
β/°	90	90	101.580(4)	101.726(2)	101.699(2)
γ/°	90	90	90	90	90
V/Å^3	3471.9(3)	3472(2)	1959.12(12)	1934.19(5)	1931.92(8)
Z	8	8	4	4	4
Z'	1	1	1	1	1
Θ_{min}/°	3.118	2.408	4.526	4.552	4.554
Θ_{max}/°	29.271	21.088	62.115	65.076	66.549
Measured Refl.	8910	8242	6804	8608	7300
Independent Refl.	3942	1873	2905	3266	3323
Reflections Used	3227	1416	2303	2818	2698
R_{int}	0.0256	0.0344	0.0848	0.0379	0.0356
Parameters	181	181	181	181	181
Restraints	0	0	0	0	0
Largest Peak	0.468	0.298	1.587	1.742	0.736
Deepest Hole	-0.393	-0.333	-1.095	-0.798	-0.796
GooF	1.033	0.948	1.056	1.067	0.956
wR_2 (all data)	0.0559	0.0689	0.1953	0.1247	0.0798
wR_2	0.0522	0.0662	0.1726	0.1193	0.0783
R_1 (all data)	0.0403	0.0391	0.0869	0.0509	0.0397
R_1	0.0280	0.0272	0.0659	0.0437	0.0315
Flack Parameter	-		-	-	-

[1] G. Scheldrick, *Acta Cryst. A* **2008**, *64*, 112-122.

[2] CrysAlisPro Software System, Agilent Technologies UK Ltd, Yarnton, Oxford, UK (different versions) **2006 - 2015**.

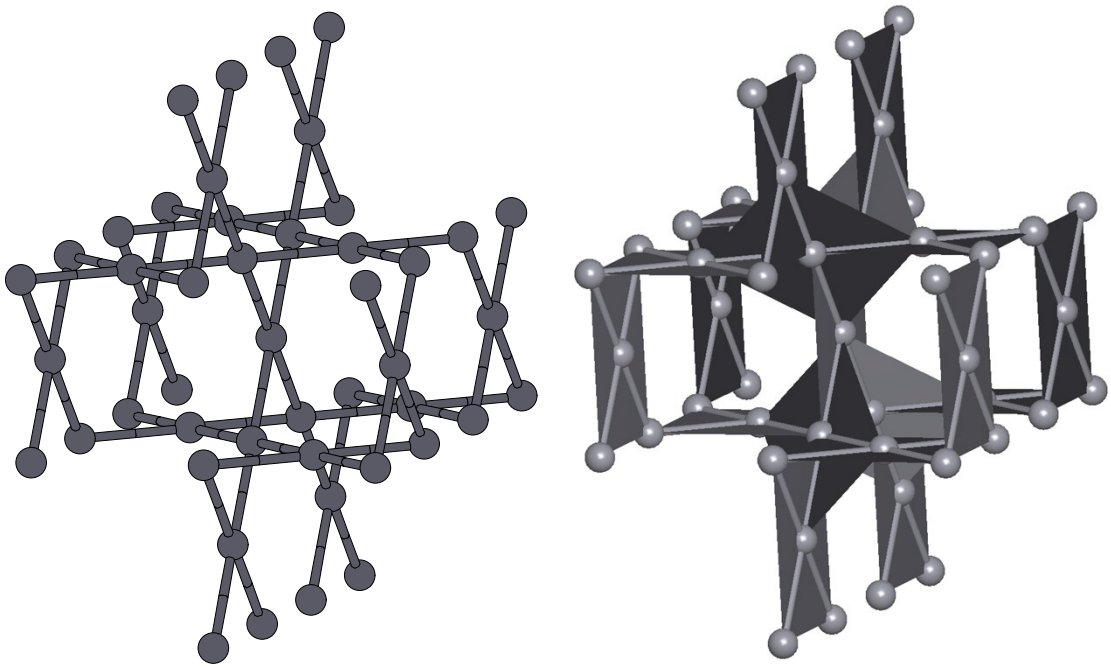
[3] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339-341.

[4] A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* **1999**, *32*, 115-119.

[5] A.L.Spek, *Acta Cryst. D* **2009**, *65*, 148-155.

Table S2. Summary of the network types and coordination environment in studied MOF

Compound	Brutto-formulae	Network	type	Coordination number of M
1	$AlCl_3bipy$	3D	lvt	6 (cation), 4 (anion)
2	$AlBr_3bipy$	2D	sql	6 (cation), 4 (anion)
3	$GaCl_3bipy$	1D		5
4	$GaBr_3bipy$	2D	sql	6 (cation), 4 (anion)
5	$GaCl_3bipy_2$	2D	sql	6 (cation), 4 (anion)



a b

Figure S1. Idealized **lvt** net, ball-and-stick (a) 'polyhedral' (b) representation

The uninodal 4-*c* 3D-net with **lvt** topology [6] is constructed from planar squares (Figure S1). Formal description of this net can be found in [7]. The **lvt** net is rather rare, taking 18th place among 20 most frequent underlying nets observed in 3D-polymeric structures containing organic ligands (see Fig. 9 in [8]). According to the TTO collection of *ToposPro* program [9], up to now there are 123 examples of compounds bearing 3D-net of this topological type. With 4,4′-bipy as a spacer only two examples of **lvt** net topology are found in CSD. Both structures are Cu(II) complexes, $(Cu_4(bipy)_8(H_2O)_6(NO_3)_2)(NO_3)_6$ (CSD: NAJMIV [10]) and $[Cu(bipy)_2(CF_3SO_3)_2]\cdot(CH_2Cl_2)$ (CSD: UFUQIV [11]), and bear only two-interpenetrated **lvt** nets. No examples with main group metals and 4,4′-bipy spacers are known.

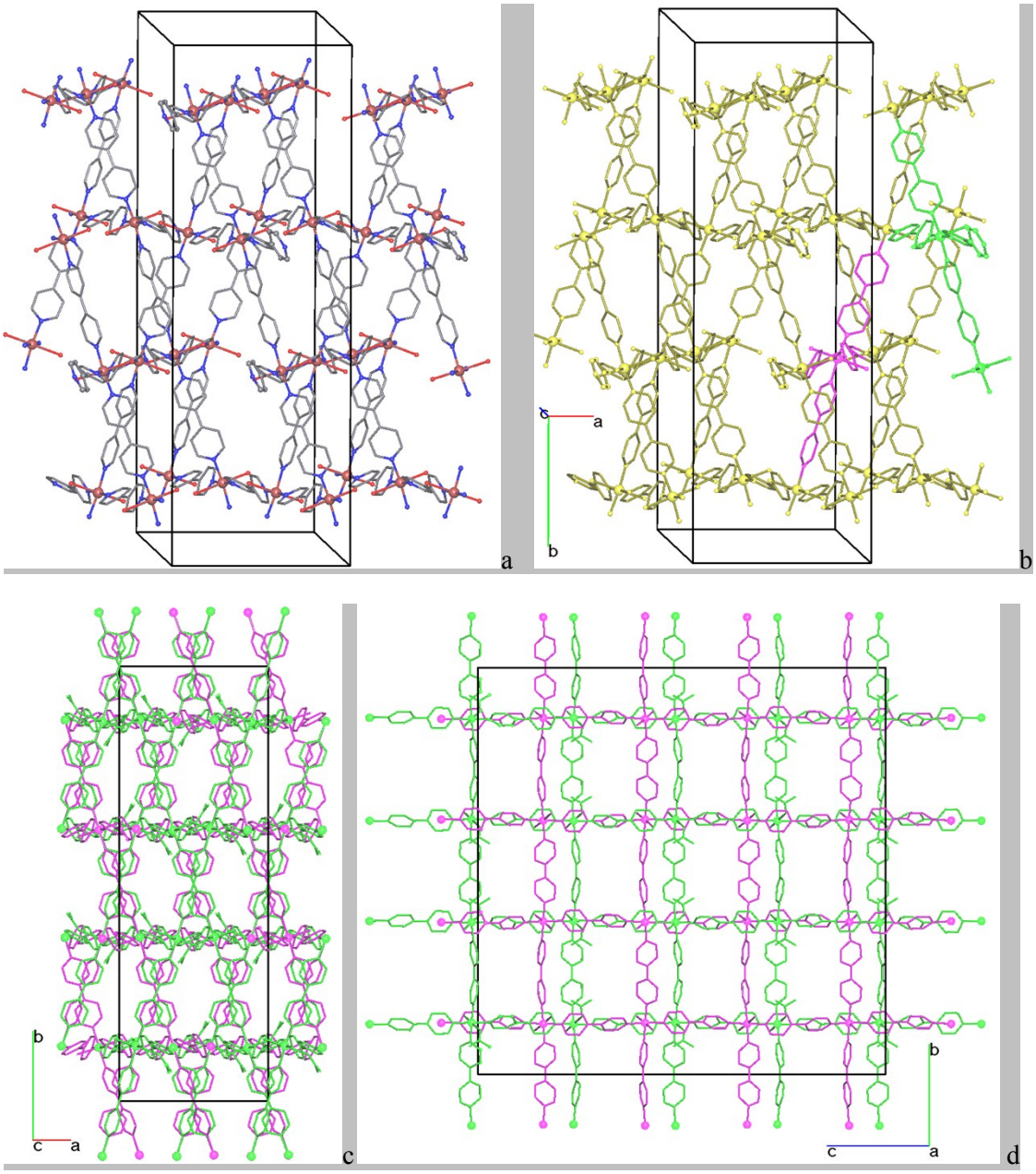


Figure S2. Crystal structure of $(Cu_4(bipy)_8(H_2O)_6(NO_3)_2)(NO_3)_6$ (CSD: NAJMIV [10]), H atoms are not shown for clarity. (a) A single framework of **lvt** topology, (b) two mutually inclined square nodes (green and magenta) formed by $Cu(bipy)_4$ units comprising the net, (c, d) veiw of two interpenetrated **lvt** frameworks.

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[7] O. Delgado Friedrichs, M. O'Keeffe, and O. M. Yaghi, Acta Cryst. (2003) A59, 515

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[9] http://topospro.com/

[10] J.Y. Lu, W.A. Fernandez ,Zhenghua Ge, K.A. Abboud. New J.Chem. (2005) V. 29 p. 434.

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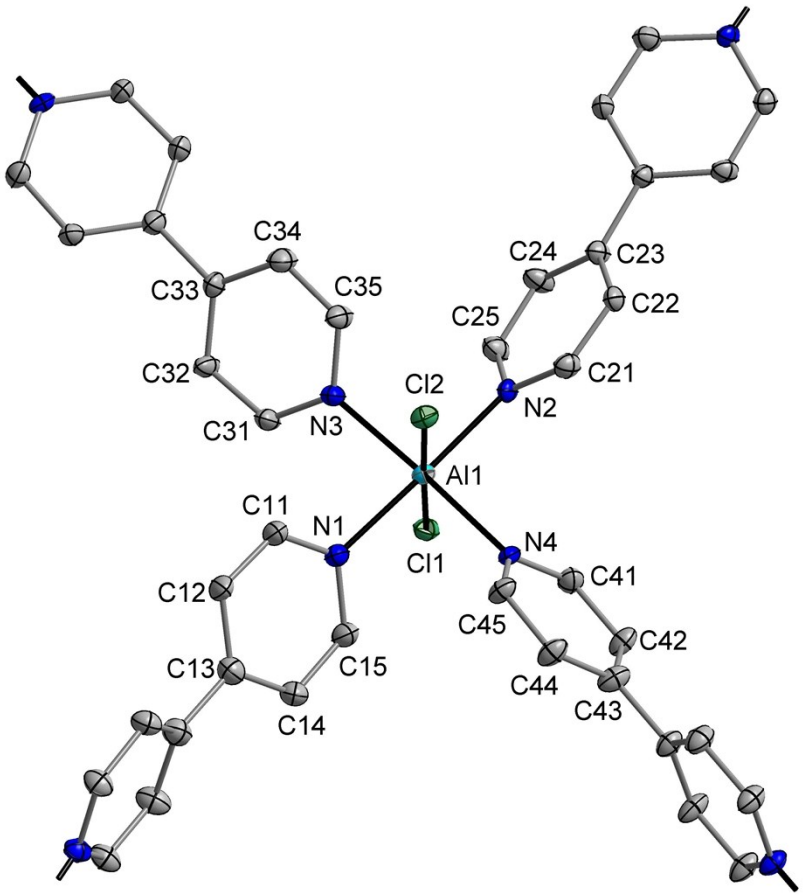


Figure S3. Section of polymeric cation in $[(AlCl_2(bipy)_2)][AlCl_4]$ (1) (ellipsoids of 50% probability) and enumerating scheme.

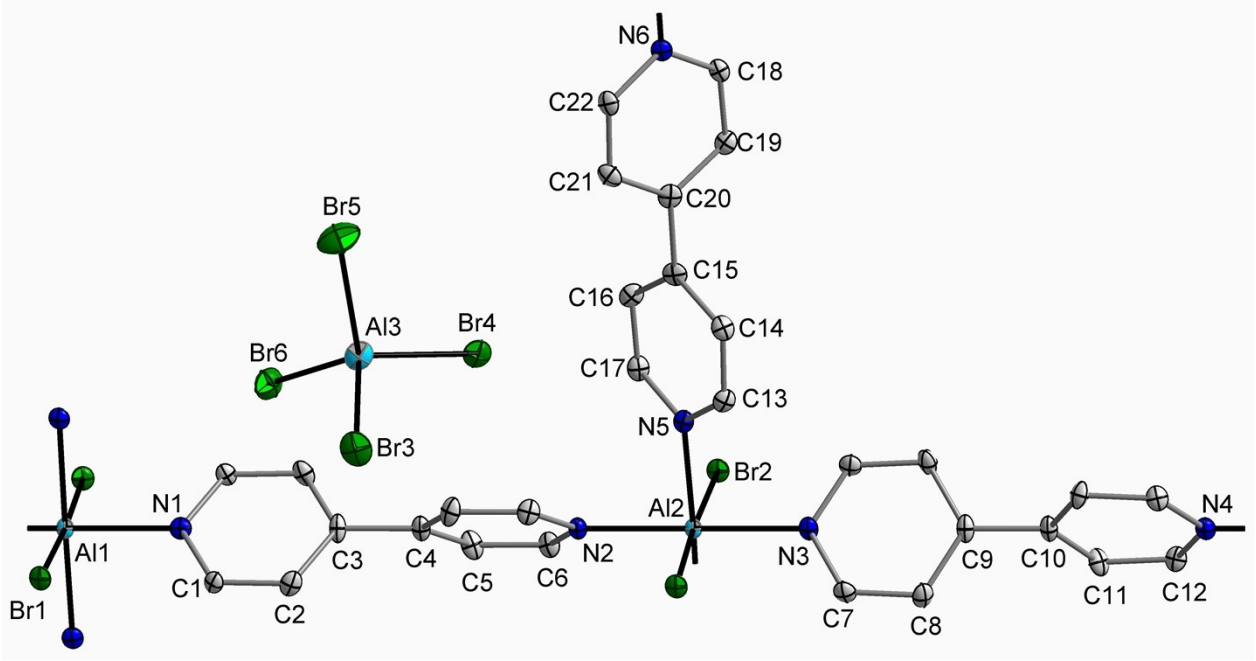
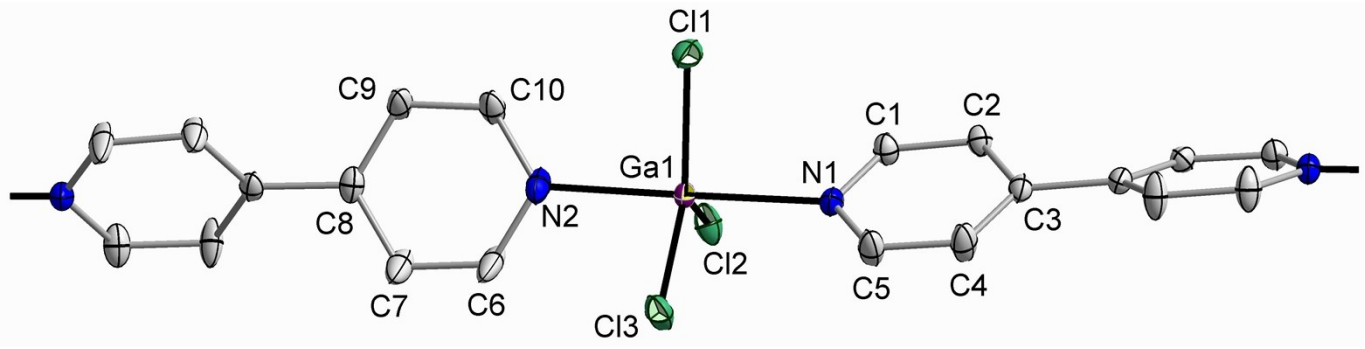
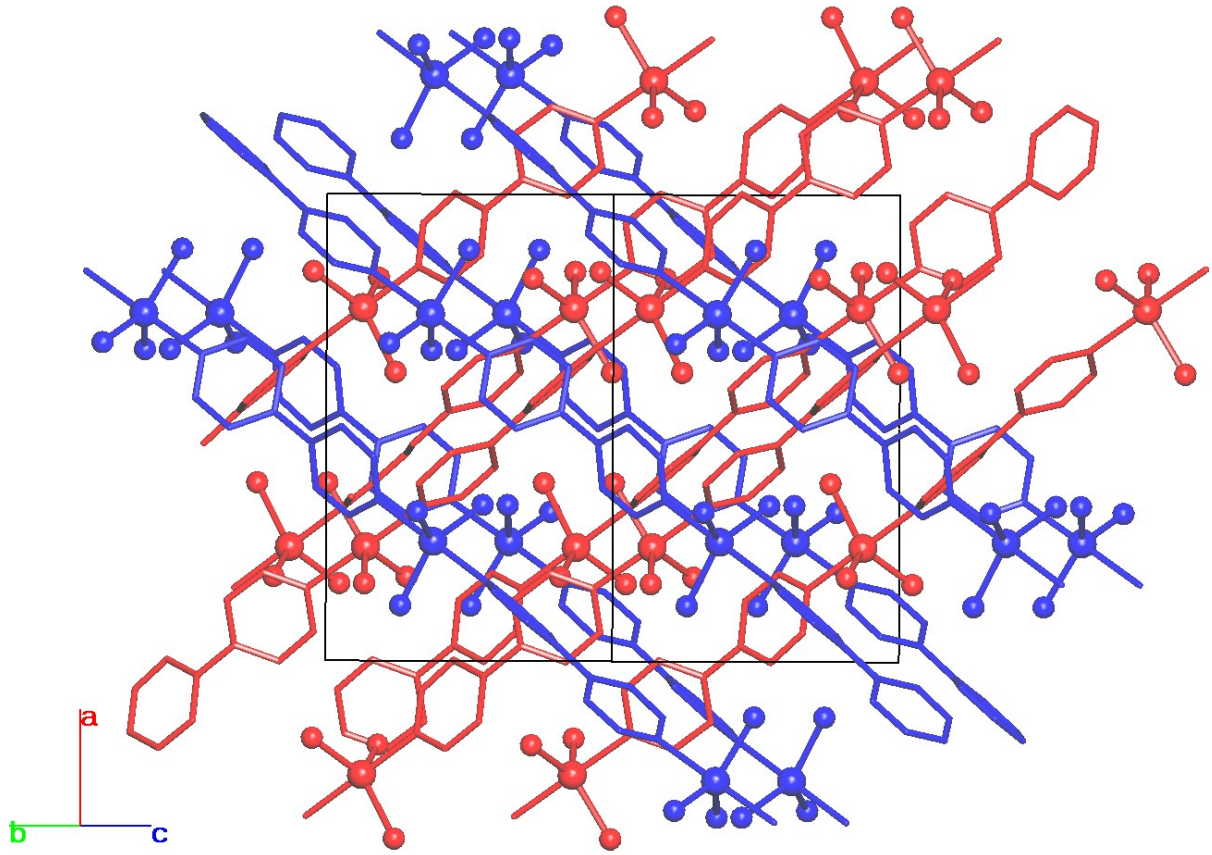


Figure S4. Section of polymeric cation in 2 (ellipsoids of 50% probability).



a



b

Figure S5. Section of chain polymer in 3 (ellipsoids of 50% probability) and enumerating scheme. (b) a packing of the chains.

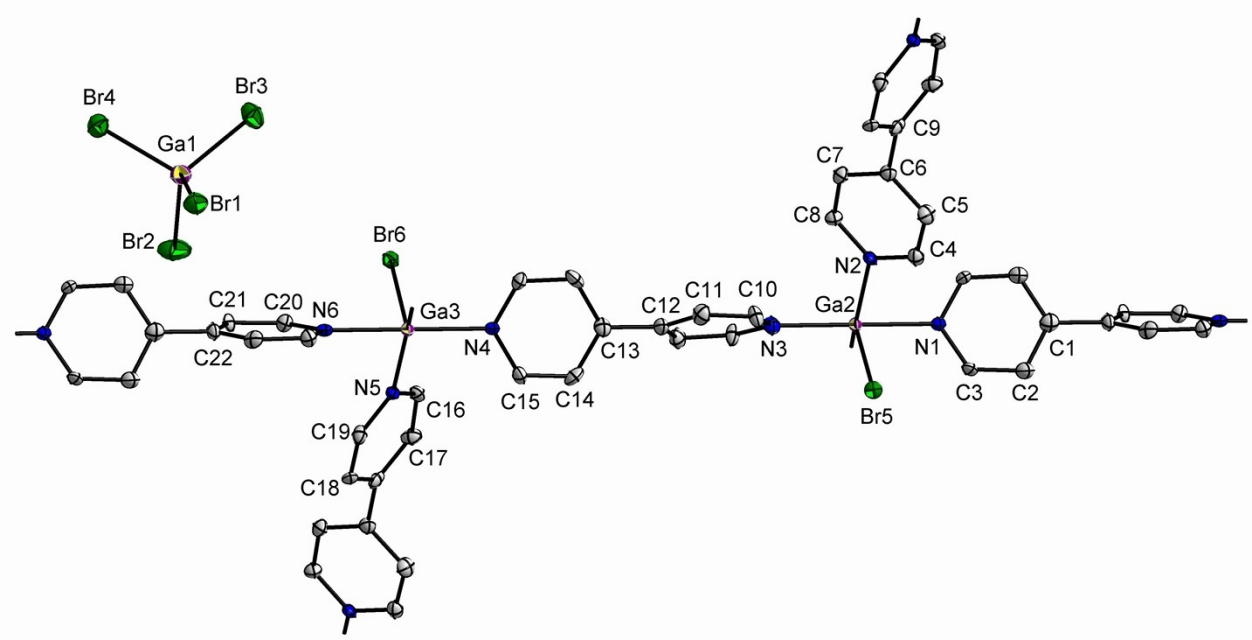
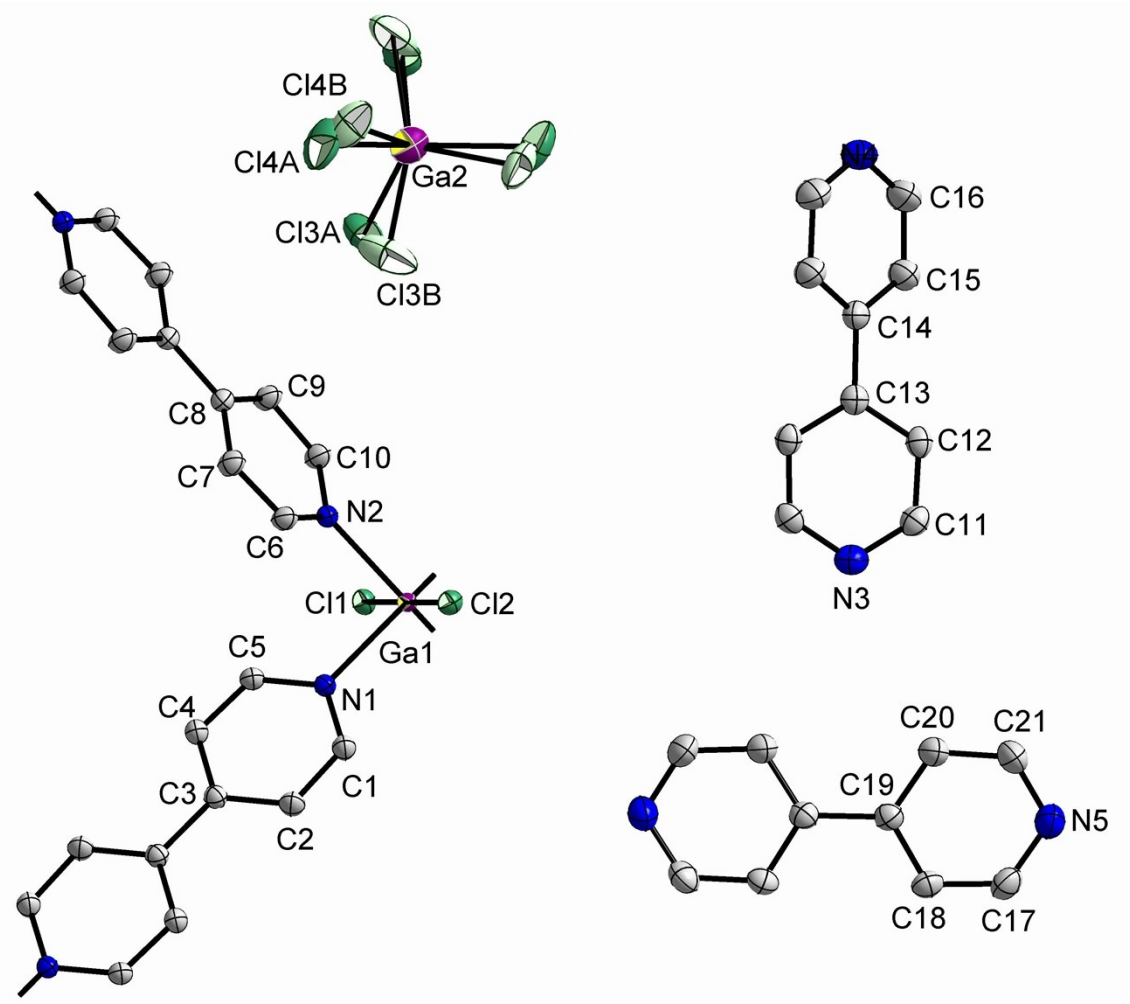


Figure S6. Section of polymeric cation in 4 (ellipsoids of 50% probability) and enumerating scheme.


Cl4B
Cl4A
Ga2
Cl3A
Cl3B
C9
C8
C10
C7
N2
C6
Cl1
Cl2
Ga1
C5
N1
C4
C1
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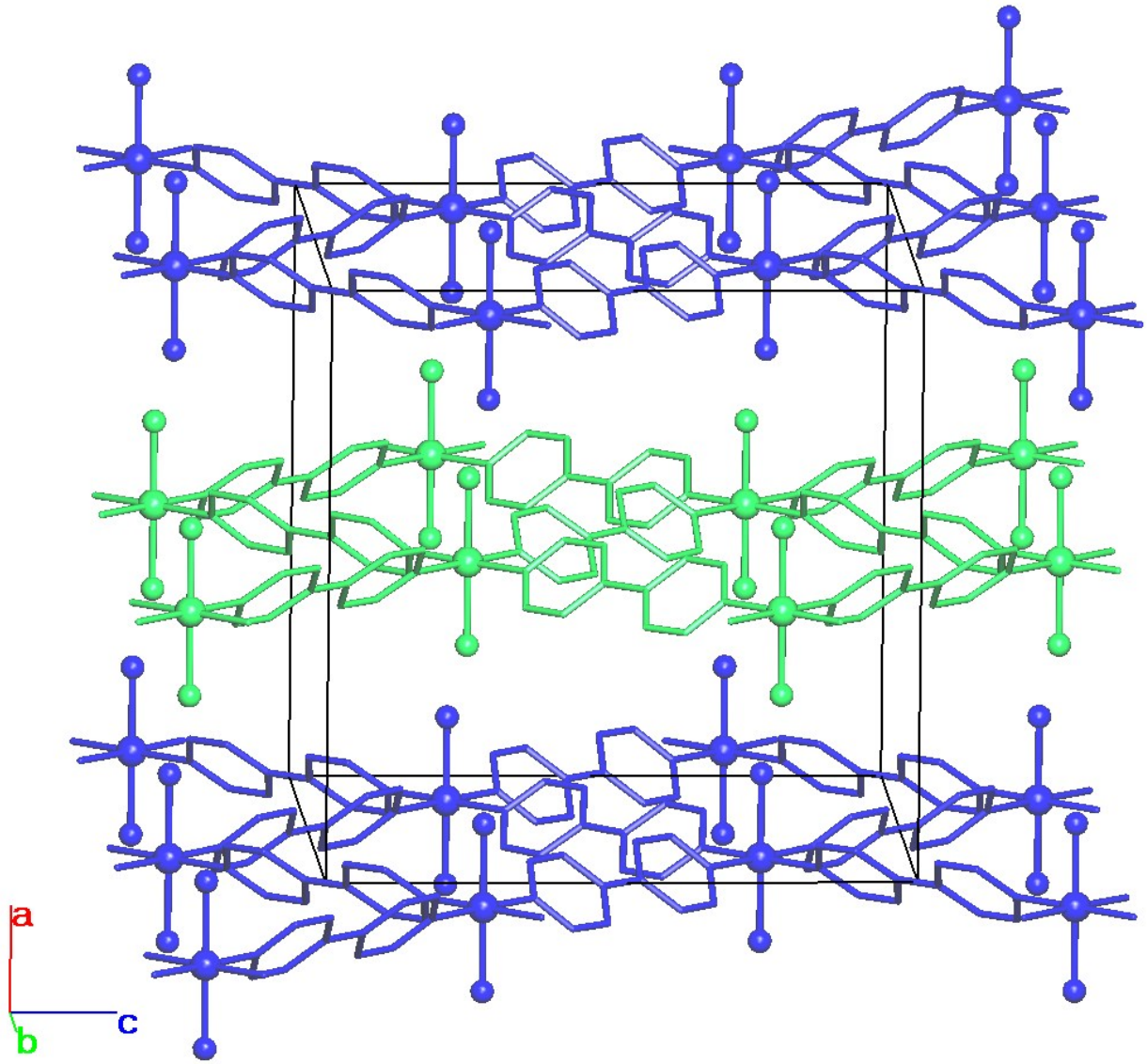
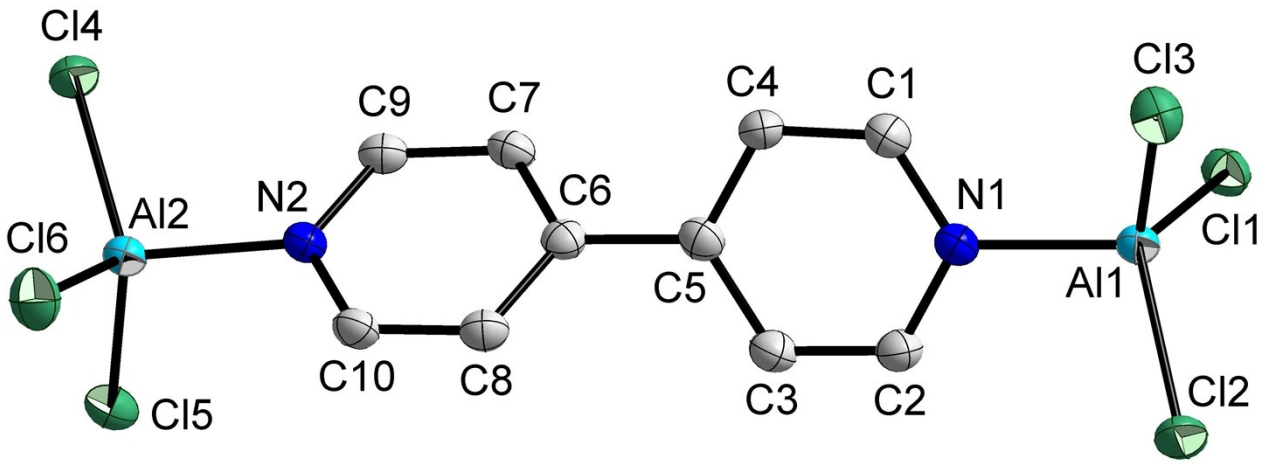
C20
C21
C19
N5
C18
C17

a

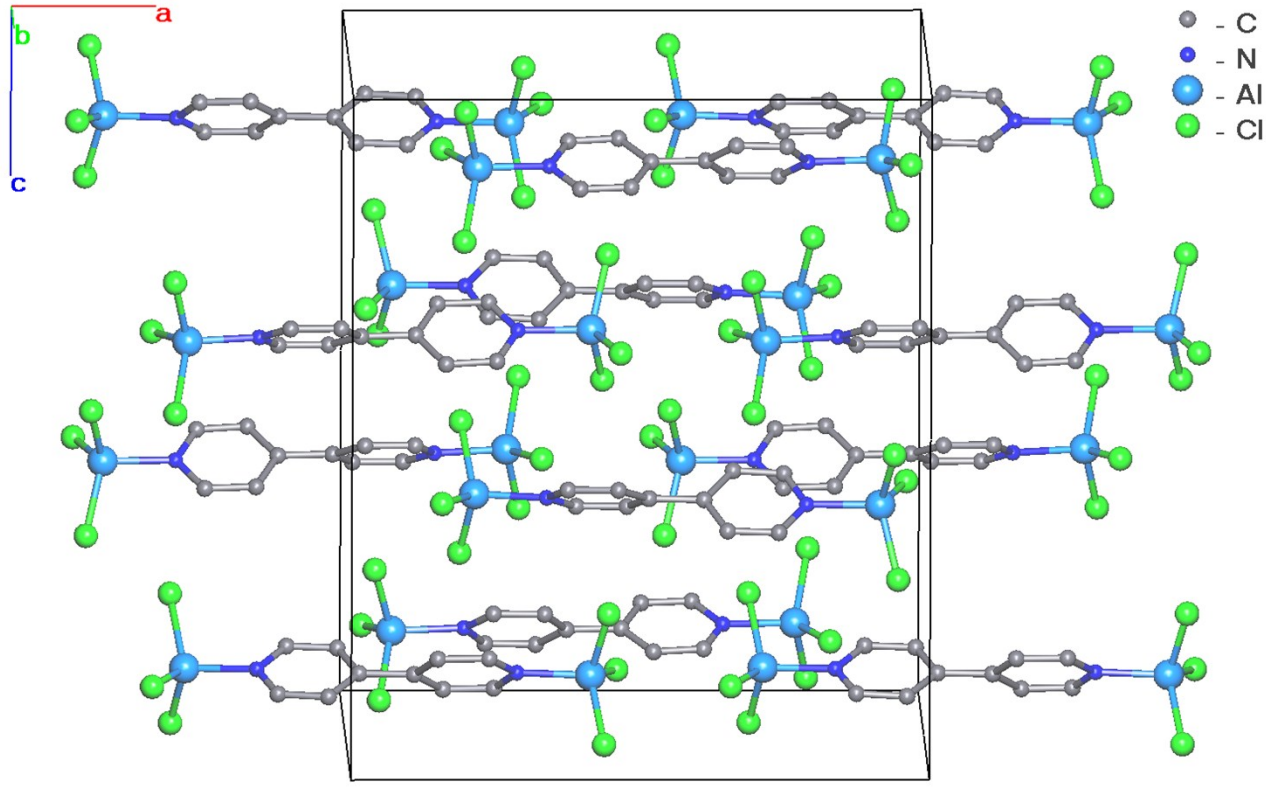


b

Figure S7. (a) The disordered anion, section of polymeric cation and co-ocrstallized bipy molecules in 5 (ellipsoids of 50% probability) and enumerating scheme. (b) the planar square nets sql in the crystal structure of 5 arranged in …ABAB… packing.



a



b

Figure S8. (a) Molecular structure in 6 (ellipsoids of 50% probability) and enumerating scheme. (b) Crystal packing of molecules for 6 in isostructural series (orthorhombic, *Pbca*) of 6-8.

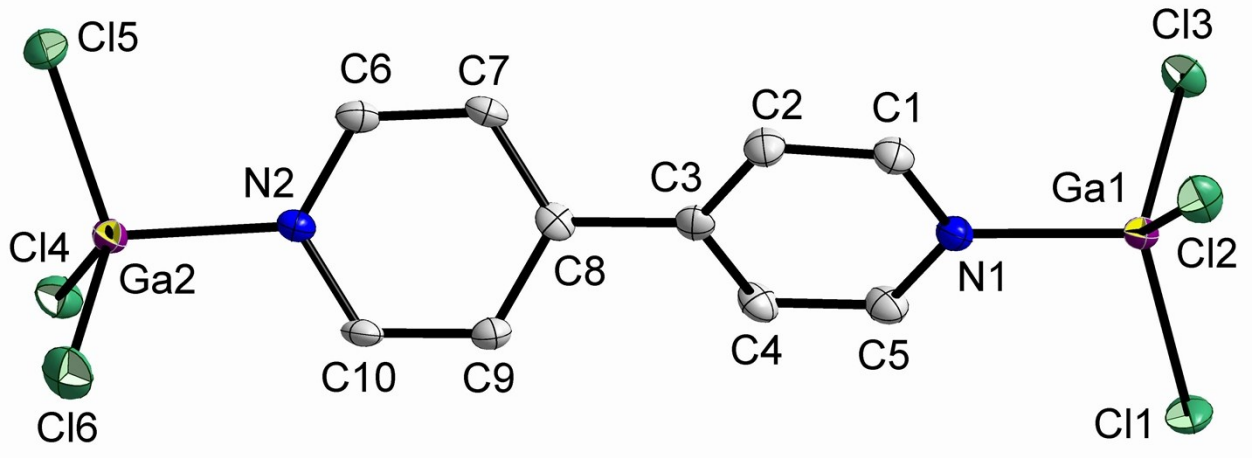


Figure S9. Molecular structure in 7 (ellipsoids of 50% probability) and enumerating scheme.

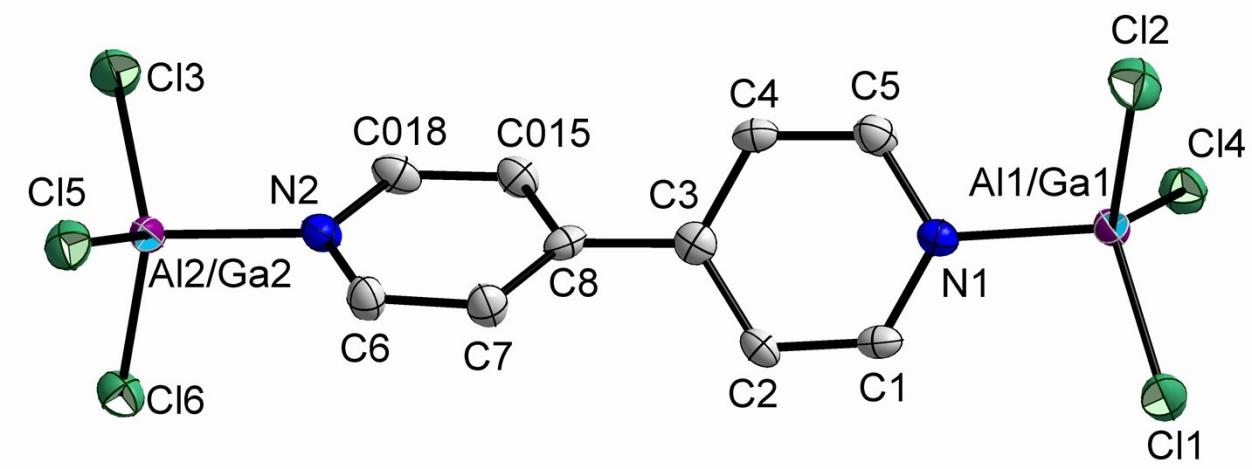
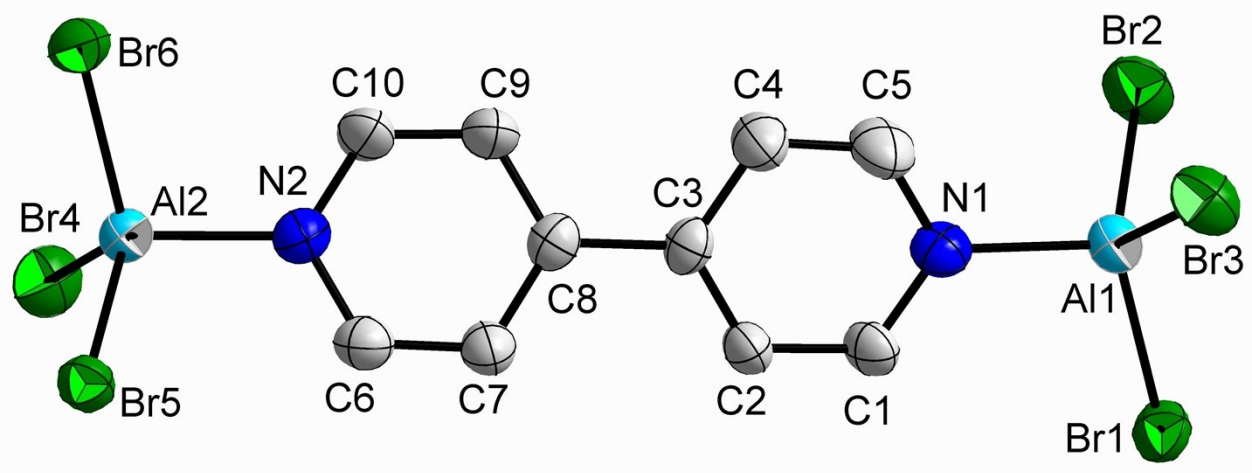
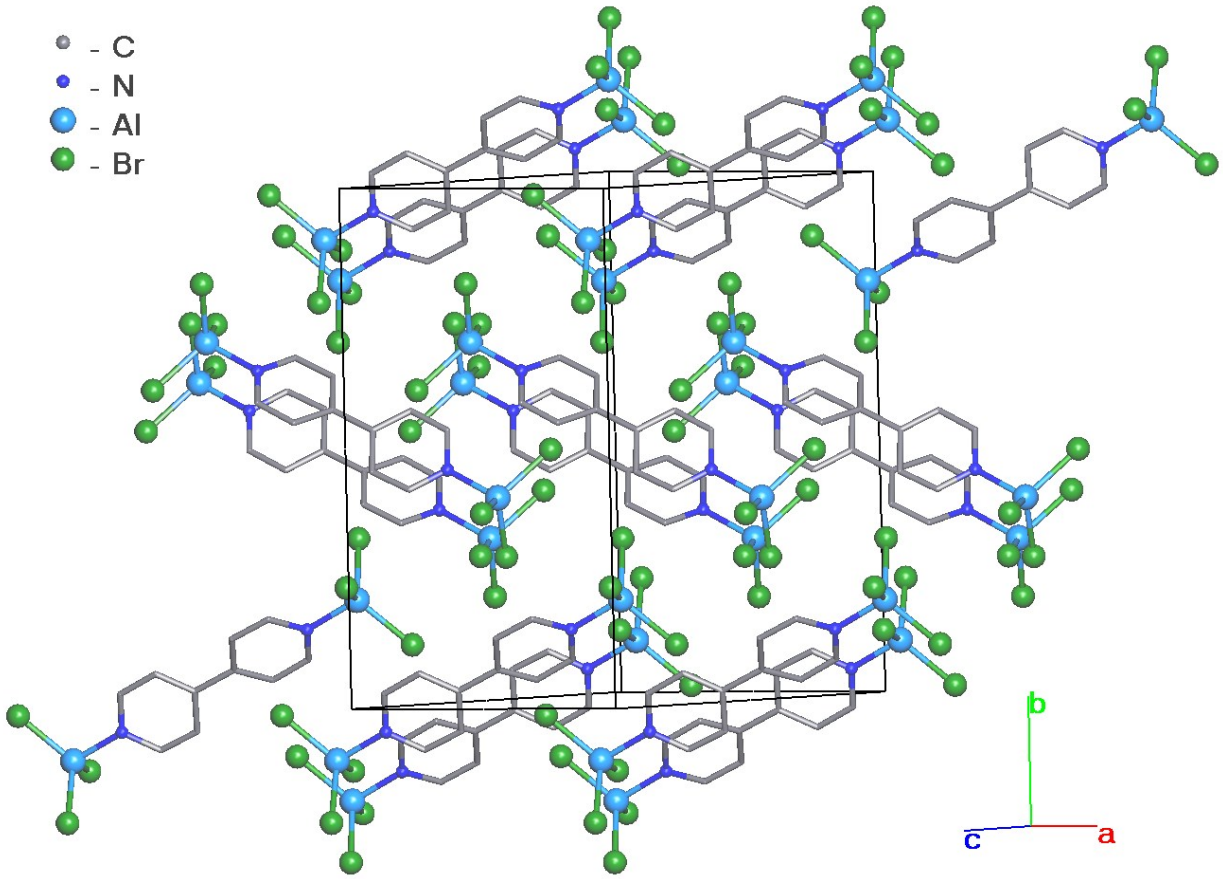


Figure S10. Molecular structure in 8 (ellipsoids of 50% probability) and enumerating scheme.



a



b

Figure S11. Molecular structure in 9 (ellipsoids of 50% probability) and enumerating scheme. (b) Crystal packing of molecules for 9 in isostructural series (monoclinic, $P2_1/c$) of 9-11.

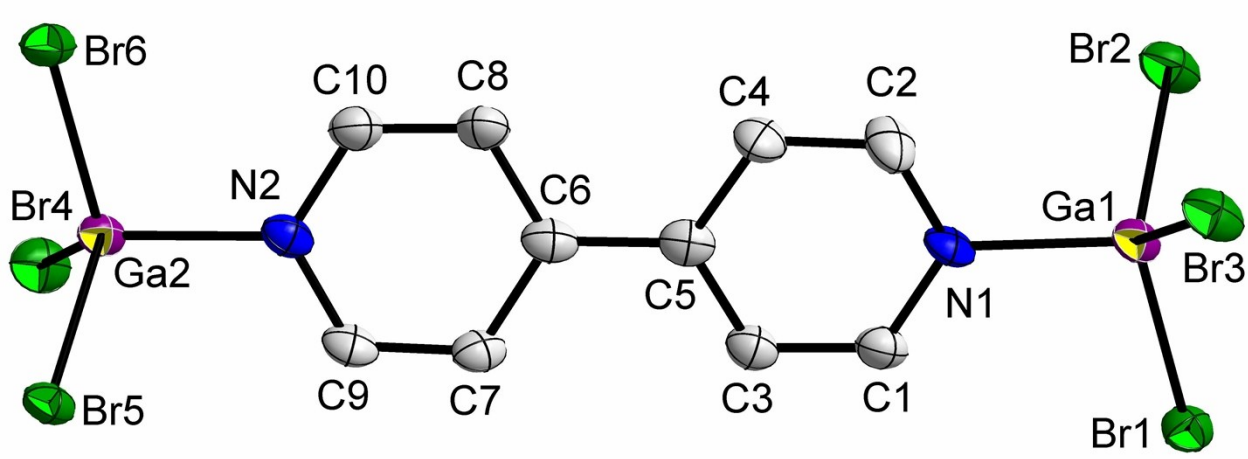


Figure S12. Molecular structure in 10 (ellipsoids of 50% probability) and enumerating scheme.

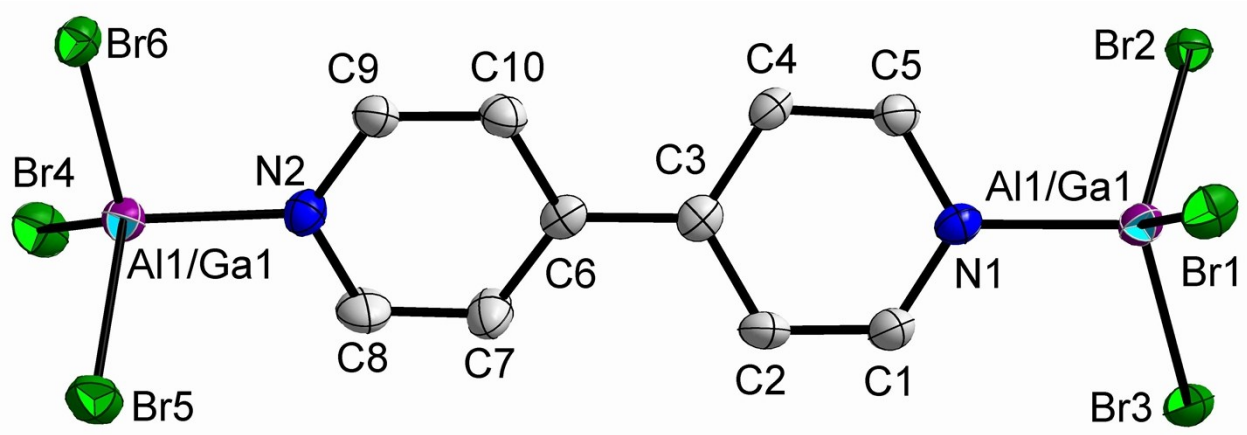


Figure S13. Molecular structure in 11 (ellipsoids of 50% probability) and enumerating scheme.

Tensimetry studies. In order to characterize the thermal stability and volatility of the complexes, a tensimetric study for the $AlBr_3$-bipy system has been carried out. The detailed description of the used static tensimetry method with glass membrane null-manometer is given elsewhere [12]. The apparatus made from quartz glass was used. Briefly, the components were stepwise introduced into the "membrane" chamber and heated up, so the synthesis of complexes occurs inside the "membrane" chamber. Two experiments have been carried out, the first in large excess of $AlBr_3$ ($AlBr_3$ to bipy ratio 4.31:1) and another one with slight excess of bipy ($AlBr_3$ to bipy ratio 1:1.02). In both experiments, formation of low volatile complexes has been evidenced. Unfortunately, the low thermal stability of **9** and low vapor pressures of **2** preclude determination of vaporization characteristics. Noticeable vapor pressure of **2** observed above 200 ºC, but above 350 ºC complex undergoes irreversible thermal destruction of the organic ligand. These data are in contrast to a tensimetric study of $GaCl_3$-pyz system [13], where the complex of 1:1 composition was more volatile and completely vaporized before the temperature of thermal destruction was reached. This behavior may be related to a non-ionic coordination polymer structure in case of $(GaCl_3pyz)_\infty$ and the ionic 2D network in case of **2**, which significantly reduces its volatility.

[12] E. I. Davydova, T. N. Sevastianova, A. V. Suvorov and A. Y. Timoshkin, *Coord. Chem. Rev.*, 2010, **254**, 2031

[13] A. Y. Timoshkin, E. A. Berezovskaya, A. V. Suvorov and A. D. Misharev, *Russ. J. Gen. Chem.*, 2005, **75**, 1173.

Mass-spectrometry studies.

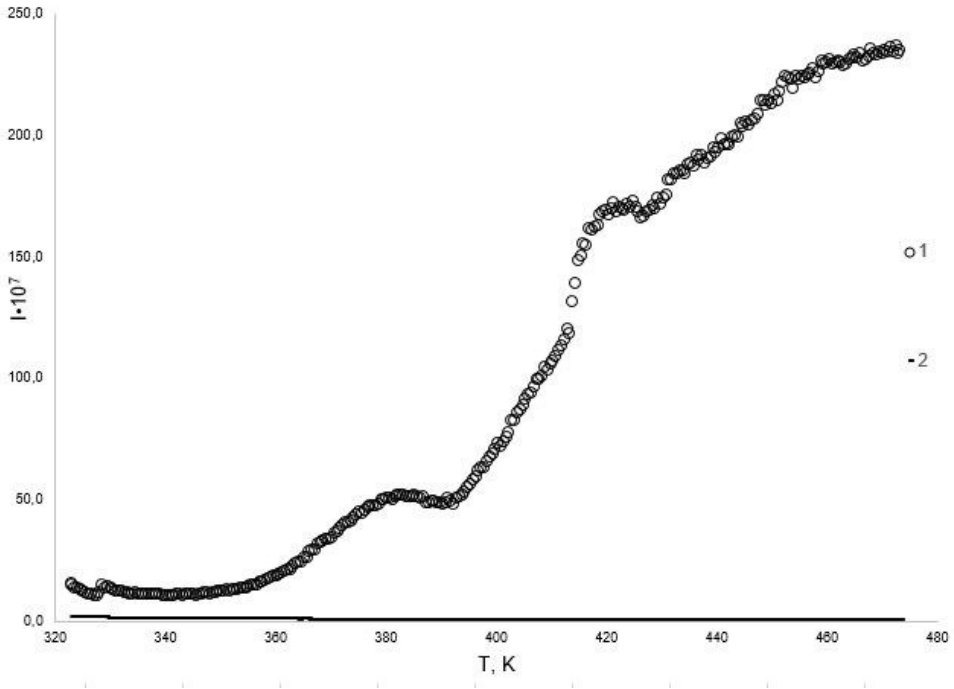


Figure S12. Dependence of the ion current (arbitrary units) of the $bipy^+$ ion from the temperature. 1 – $bipy^+$ above **5**, 2 – $bipy^+$ above **3**.

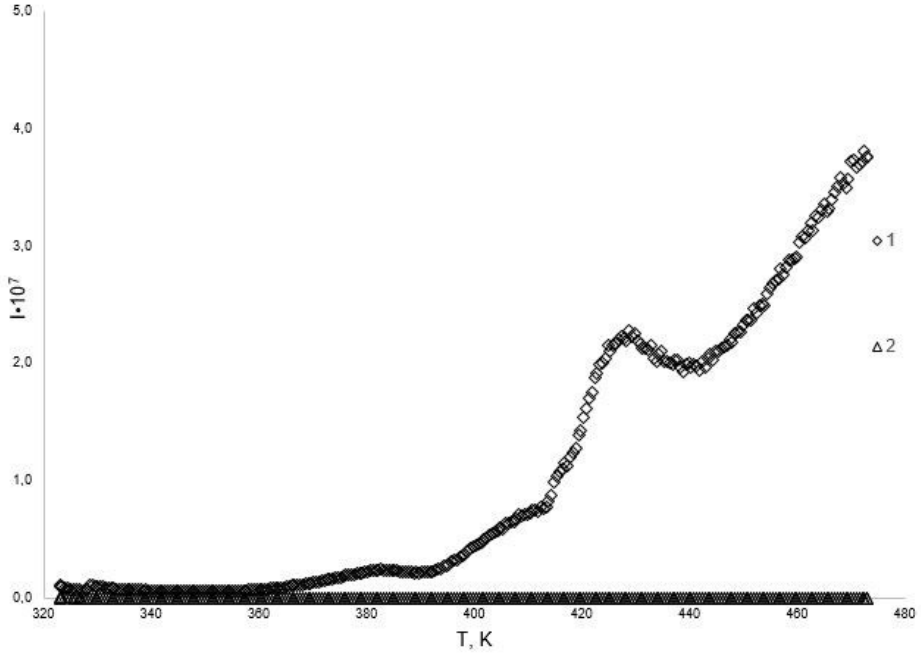


Figure S15. Dependence of the ion current (arbitrary units) of the $GaCl_2bipy^+$ ion from the temperature. 1 – $GaCl_2bipy^+$ above **5**, 2 – $GaCl_2bipy^+$ above **3**.

TG measurements for vapor pressure determination above 5.

Vapor pressure determinations were carried out under stationary mass transfer conditions with heating rate of 1K per minute. Knudsen cell with orifice diameter 1.0-1.1 mm was used. Naphthalene (Sigma, 99%) was used as reference compound. The used temperature program is given in Table S3.

Table S3. Temperature program used for TG experiment.

Num	Mode	Temp. °C	HR K/min	Acq.Rate pts/min	Duration hh:mm	STC	P1:Ar	PG:Ar	Vac
---	Stand-by heating	40.0	5.000	0x E+F		0	50.0	50.0	0
---	Stand-by isothermal	40.0			00:10	0	50.0	50.0	0
1	Dynamic	130.0	20.000	600.00	00:05	0	50.0	50.0	0
2	Isothermal	130.0		300.00	00:15	0	50.0	50.0	0
3	Dynamic	190.0	1.000	300.00	01:00	0	50.0	50.0	0
4	Dynamic	130.0	10.000	300.00	00:06	0	50.0	50.0	0
5	Isothermal	130.0		300.00	00:05	0	50.0	50.0	0
6	Dynamic	190.0	1.000	300.00	01:00	0	50.0	50.0	0
7	Dynamic	40.0	10.000	300.00	00:15	0	50.0	50.0	0
8	Isothermal	40.0		300.00	00:10	0	50.0	50.0	0
---	Emergency	200.0					0.0	0.0	0
---	Final stand-by heating	40.0	10.000		00:00	0	50.0	50.0	0
---	Final stand-by isothermal	40.0			00:10	0	0.0	0.0	0

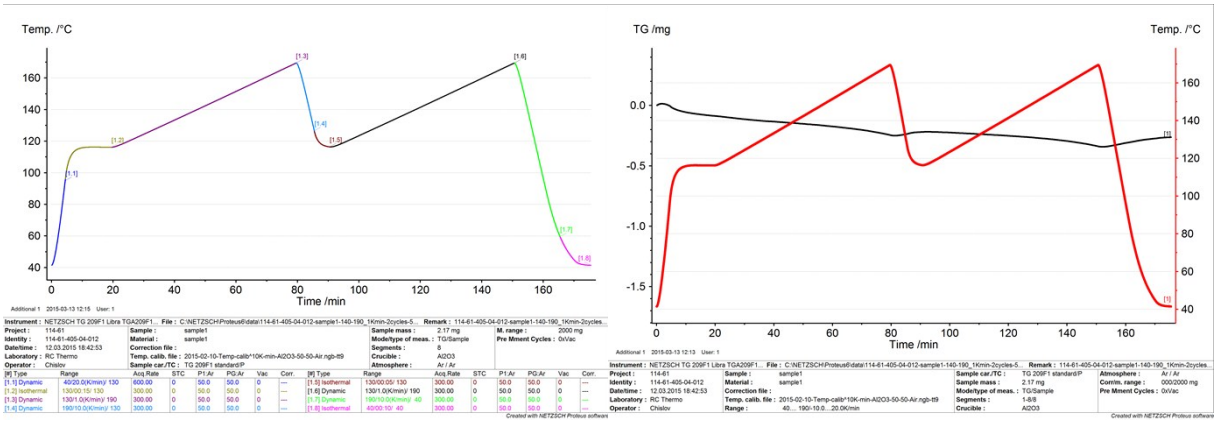
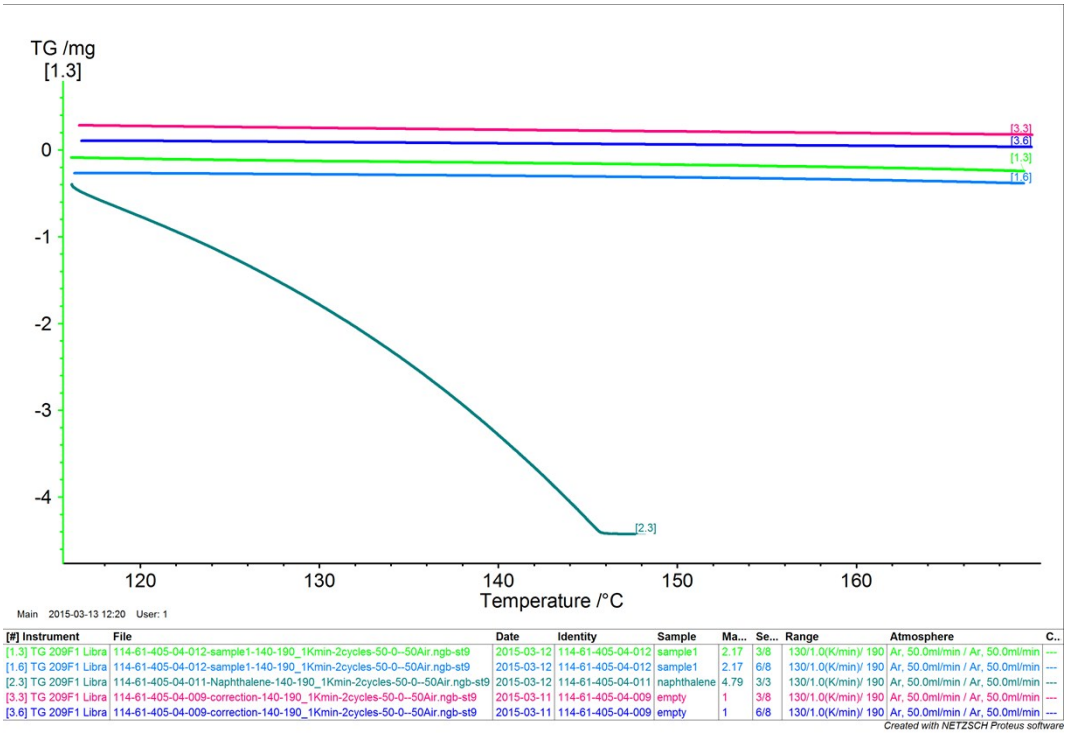


Figure S16. Graphical representation of the temperature program.



[#] Instrument	File	Date	Identity	Sample	Ma...	Se...	Range	Atmosphere	C..
[1.3] TG 209F1 Libra	114-61-405-04-012-sample1-140-190_1Kmin-2cycles-50-0--50Air.ngb-st9	2015-03-12	114-61-405-04-012	sample1	2.17	3/8	130/1.0(K/min)/ 190	Ar, 50.0ml/min / Ar, 50.0ml/min	---
[1.6] TG 209F1 Libra	114-61-405-04-012-sample1-140-190_1Kmin-2cycles-50-0--50Air.ngb-st9	2015-03-12	114-61-405-04-012	sample1	2.17	6/8	130/1.0(K/min)/ 190	Ar, 50.0ml/min / Ar, 50.0ml/min	---
[2.3] TG 209F1 Libra	114-61-405-04-011-Naphthalene-140-190_1Kmin-2cycles-50-0--50Air.ngb-st9	2015-03-12	114-61-405-04-011	naphthalene	4.79	3/3	130/1.0(K/min)/ 190	Ar, 50.0ml/min / Ar, 50.0ml/min	---
[3.3] TG 209F1 Libra	114-61-405-04-009-correction-140-190_1Kmin-2cycles-50-0--50Air.ngb-st9	2015-03-11	114-61-405-04-009	empty	1	3/8	130/1.0(K/min)/ 190	Ar, 50.0ml/min / Ar, 50.0ml/min	---
[3.6] TG 209F1 Libra	114-61-405-04-009-correction-140-190_1Kmin-2cycles-50-0--50Air.ngb-st9	2015-03-11	114-61-405-04-009	empty	1	6/8	130/1.0(K/min)/ 190	Ar, 50.0ml/min / Ar, 50.0ml/min	---

Created with NETZSCH Proteus software

Figure S17. Obtained TG results.

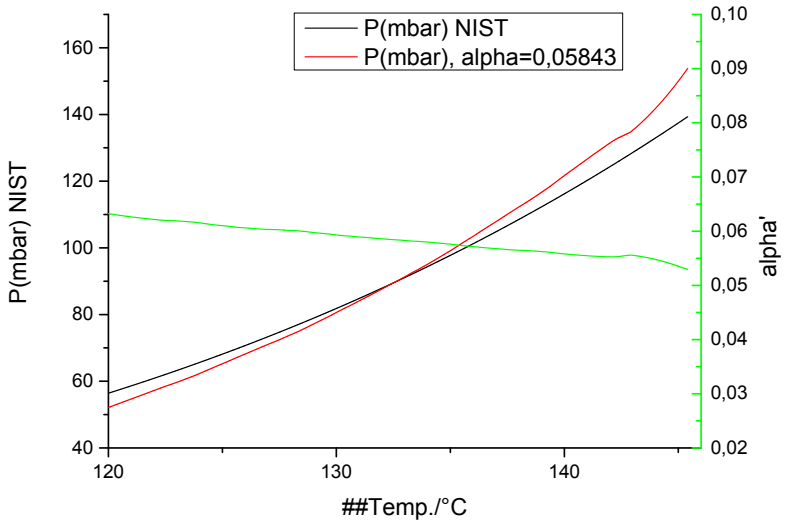


Figure S18. Vapor pressure-temperature dependence of naphthalene, computed using NIST values, and experimental vapor pressure obtained with α=0.05843.

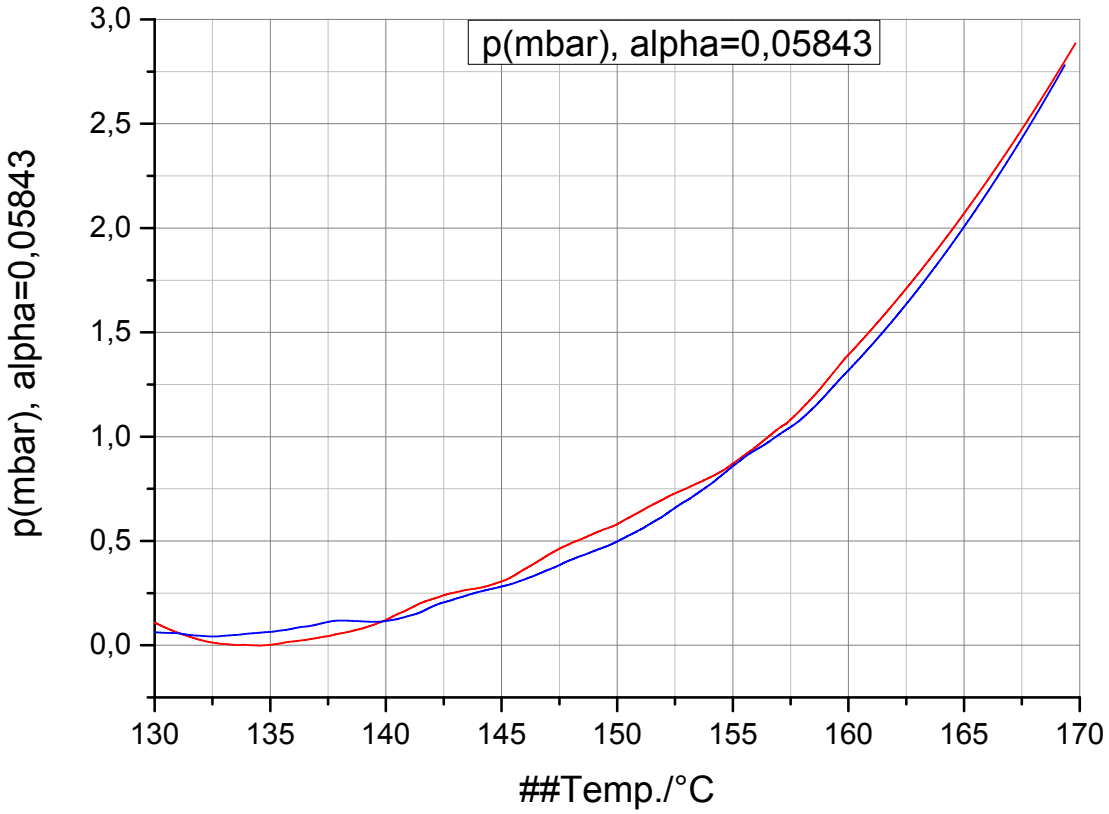
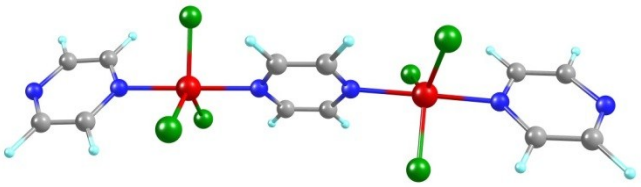


Figure S19. Vapor-pressure temperature dependence over **5** obtained in two independent experiments using α=0.05843.

Computational studies.

Table S4. Optimized structures and xyz coordinates for considered compounds. RI-BP86/def2-SVP level of theory.

$(AlCl_3)_2pyz_3$ (staggered, C_2)

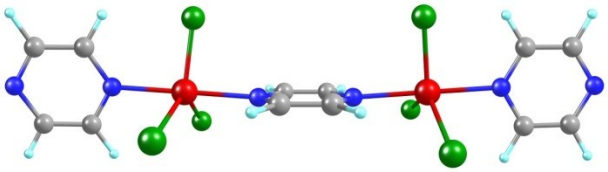


E = -4038.387520032

	X	Y	Z
Cl	-3.3643527	0.9167302	1.9103070
Al	-3.5845906	0.0028480	-0.0625326
Cl	-3.7219165	-2.1659317	-0.2738245
Cl	-3.5764565	1.2839919	-1.8332315
N	-5.7338040	0.0753204	0.0541739
N	-1.3985424	-0.0458664	-0.1663961
N	1.3985424	0.0458664	-0.1663961
C	-0.7366085	1.1288447	-0.1727234
C	-0.6629461	-1.1762503	-0.1712345
C	0.7366085	-1.1288447	-0.1727234
C	0.6629461	1.1762503	-0.1712345
H	-1.3408331	2.0476679	-0.1837850
H	-1.2233446	-2.1240452	-0.1745846
H	1.3408331	-2.0476679	-0.1837850
H	1.2233446	2.1240452	-0.1745846
N	-8.5415272	-0.0691090	0.1721274
C	-6.4847076	0.0891272	-1.0685887
C	-6.3824800	-0.0055442	1.2355866
C	-7.7840970	-0.0781023	1.2798897
C	-7.8844989	0.0155276	-0.9955171
H	-5.9431373	0.1785223	-2.0225705
H	-5.7563326	0.0056474	2.1409452
H	-8.3028026	-0.1424263	2.2516210
H	-8.4869756	0.0293524	-1.9196622
Cl	3.7219165	2.1659317	-0.2738245
Al	3.5845906	-0.0028480	-0.0625326
Cl	3.3643527	-0.9167302	1.9103070
Cl	3.5764565	-1.2839919	-1.8332315
N	5.7338040	-0.0753204	0.0541739
N	8.5415272	0.0691090	0.1721274
C	6.4847076	-0.0891272	-1.0685887
C	6.3824800	0.0055442	1.2355866
C	7.7840970	0.0781023	1.2798897
C	7.8844989	-0.0155276	-0.9955171
H	5.9431373	-0.1785223	-2.0225705
H	5.7563326	-0.0056474	2.1409452
H	8.3028026	0.1424263	2.2516210
H	8.4869756	-0.0293524	-1.9196622

$(AlCl_3)_2pyz_3$ (eclipsed, C_2)

	X	Y	Z
Cl	3.3146671	-0.2554357	2.1145718
Al	3.5873508	-0.0376597	-0.0402006
Cl	3.7311451	1.9437406	-0.9509106



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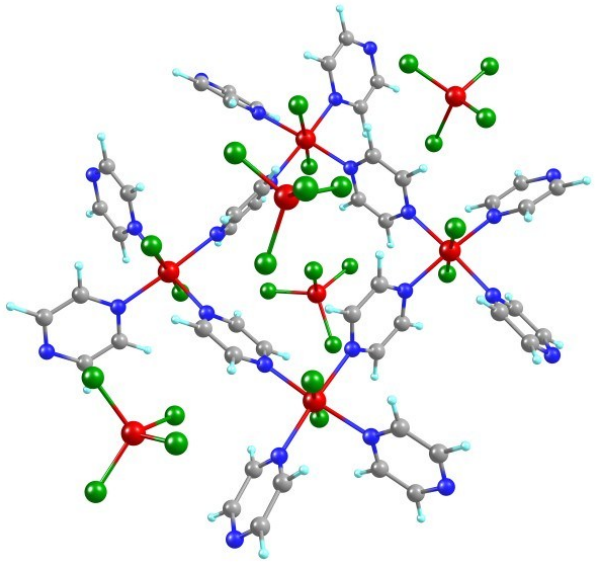
N	-1.4005165	0.0011654	-0.1975966
C	0.6987980	-1.1531520	-0.1982899
C	0.7015730	1.1524655	-0.1982946
C	-0.6987980	1.1531520	-0.1982899
C	-0.7015730	-1.1524655	-0.1982946
H	1.2785736	-2.0878125	-0.2253887
H	1.2882196	2.0834777	-0.2222158
H	-1.2785736	2.0878125	-0.2253887
H	-1.2882196	-2.0834777	-0.2222158
N	8.5456783	0.0009109	0.1463466
C	6.4543854	-0.1283672	-1.0371236
C	6.4140103	0.0129956	1.2666494
C	7.8191644	0.0497762	1.2723578
C	7.8556367	-0.0884998	-1.0030735
H	5.8922836	-0.2143616	-1.9790251
H	5.8070672	0.0477010	2.1849256
H	8.3649193	0.1208195	2.2287108
H	8.4330841	-0.1321424	-1.9420986
Cl	-3.7311451	-1.9437406	-0.9509106
Al	-3.5873508	0.0376597	-0.0402006
Cl	-3.3146671	0.2554357	2.1145718
Cl	-3.6453422	1.8067096	-1.3244433
N	-5.7337990	0.0748779	0.1050990
N	-8.5456783	-0.0009109	0.1463466
C	-6.4543854	0.1283672	-1.0371236
C	-6.4140103	-0.0129956	1.2666494
C	-7.8191644	-0.0497762	1.2723578
C	-7.8556367	0.0884998	-1.0030735
H	-5.8922836	0.2143616	-1.9790251
H	-5.8070672	-0.0477010	2.1849256
H	-8.3649193	-0.1208195	2.2287108
H	-8.4330841	0.1321424	-1.9420986

$[Al_4Cl_8pyz_{12}]^{4+}([AlCl_4]^-)_4$ (C_1)

	X	Y	Z
N	-6.7412778	1.3105856	0.0208569
Al	-5.0341089	0.0726855	-0.0343684
N	-3.3246054	-1.3245270	-0.1351938
N	-3.6735221	1.7113878	-0.0728281
N	-6.3432412	-1.7015976	-0.0175714
Cl	-5.1778937	0.0534608	-2.2962616
N	-1.6783808	3.6989106	-0.0912870
C	-3.4741080	2.5207627	0.9920104
C	-2.9122408	1.9433315	-1.1662997
C	-1.9228426	2.9285102	-1.1758753
C	-2.4795948	3.5137219	0.9823767
H	-4.1037750	2.3691413	1.8791096



E = -16153.52713732

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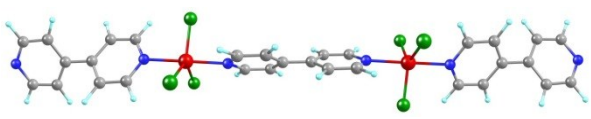
H	-2.3194336	4.1517580	1.8622390
Al	-0.0282253	5.0336077	-0.0815625
N	-1.3315217	-3.3216293	-0.1765373
C	-2.5001655	-1.5226214	0.9182072
C	-3.0906945	-2.0744242	-1.2370054
C	-2.1023241	-3.0645430	-1.2592634
C	-1.5065163	-2.5188196	0.8977637
H	-2.6561566	-0.9188994	1.8257679
H	-3.7156365	-1.8721353	-2.1189846
H	-1.9159130	-3.6654782	-2.1609524
H	-0.8819928	-2.6934764	1.7880361
Al	0.0559730	-5.0383204	-0.1448260
N	1.7695835	6.3304629	-0.0973366
N	-1.2215157	6.7569457	0.0376582
N	1.3255225	3.3108679	-0.2357754
Cl	-0.0438721	5.1917995	-2.3403613
Cl	0.1522853	4.9308440	2.1496382
N	1.2692677	-6.7713702	-0.1518672
N	1.6868128	-3.6694749	-0.2129979
N	-1.7430855	-6.3134714	-0.0815268
Cl	-0.0083577	-5.1547888	-2.3975103
Cl	0.0590231	-5.0228490	2.0929667
N	3.6666650	-1.6740983	-0.2112769
C	2.5793011	-3.5653625	0.7946127
C	1.8226496	-2.8075426	-1.2489544
C	2.8090150	-1.8171670	-1.2495752
C	3.5666955	-2.5657236	0.7975386
H	2.4983043	-4.2745346	1.6300966
H	1.1260974	-2.9036041	-2.0959609
H	2.9012173	-1.1195672	-2.0963580
H	4.2728856	-2.4831596	1.6353905
Al	5.0290006	-0.0465913	-0.1518456
N	3.3149367	1.3204728	-0.2589267
C	1.4004098	2.3786003	0.7405045
C	2.1805173	3.1763875	-1.2744626
C	3.1696823	2.1858427	-1.2877257
C	2.3941516	1.3855035	0.7288376
H	0.6801965	2.4258718	1.5745365
H	2.0602968	3.8800647	-2.1110344
H	3.8614231	2.0733166	-2.1348984
H	2.4501387	0.6530542	1.5515095
N	6.3327015	1.7401239	-0.1045843
N	6.7581433	-1.2493052	-0.0603600
Cl	5.1899477	-0.0224162	-2.3999240
Cl	4.9213577	0.0449125	2.0866491
N	8.0547993	3.9727863	-0.0091321
C	6.2817561	2.6293143	0.9136897

C	7.2473724	1.9692591	-1.0743393
C	8.1055220	3.0801403	-1.0098753
C	7.1390024	3.7414382	0.9441066
H	5.5646952	2.4096495	1.7197121
H	7.2629978	1.2563628	-1.9126558
H	8.8551106	3.2441253	-1.8025421
H	7.0815344	4.4586970	1.7805175
N	9.1825301	-2.6858797	-0.0658138
C	7.6938271	-1.0636374	0.9018186
C	7.0081175	-2.2073682	-0.9813787
C	8.2146419	-2.9291379	-0.9594041
C	8.9044750	-1.7690970	0.8732558
H	7.4507958	-0.3441485	1.6968002
H	6.2464848	-2.3839573	-1.7512663
H	8.3895417	-3.7229976	-1.7038503
H	9.6712171	-1.5762808	1.6424407
N	2.6724966	-9.2083686	-0.3286689
C	1.0792294	-7.7647480	0.7492259
C	2.2195704	-6.9712027	-1.0922626
C	2.9240791	-8.1858093	-1.1559236
C	1.7678770	-8.9802316	0.6354267
H	0.3673233	-7.5657274	1.5631714
H	2.4015628	-6.1633392	-1.8123596
H	3.7065935	-8.3212318	-1.9205063
H	1.5690980	-9.7938555	1.3532542
N	-4.0306141	-7.9619379	0.0170121
C	-2.6005830	-6.2710852	0.9647277
C	-2.0310167	-7.1836564	-1.0765162
C	-3.1690355	-8.0052644	-1.0107707
C	-3.7401282	-7.0915783	0.9964527
H	-2.3377529	-5.5903161	1.7893840
H	-1.3433331	-7.1919549	-1.9356604
H	-3.3820434	-8.7175336	-1.8258402
H	-4.4309400	-7.0409010	1.8551123
N	-8.0469778	-3.9489071	0.0350172
C	-6.2763004	-2.6159280	0.9773622
C	-7.2655662	-1.9119867	-0.9841783
C	-8.1149923	-3.0302807	-0.9407636
C	-7.1240846	-3.7356485	0.9856074
H	-5.5543665	-2.4137356	1.7834937
H	-7.2946677	-1.1797078	-1.8048471
H	-8.8711901	-3.1791468	-1.7301886
H	-7.0521471	-4.4749728	1.8012576
N	-2.6899425	9.1600123	0.0846887
C	-2.2210373	6.9891082	-0.8426340
C	-1.0041601	7.7007215	0.9854413
C	-1.7270399	8.9010815	0.9825232
C	-2.9577315	8.1853819	-0.7941313
H	-2.4165870	6.2231157	-1.6036077

H	-0.2468564	7.4711302	1.7485472
H	-1.5109753	9.6750430	1.7379841
H	-3.7833166	8.3466571	-1.5063644
N	4.0309897	8.0170941	-0.0896447
C	2.7082285	6.2503114	0.8733763
C	1.9626459	7.2585566	-1.0621756
C	3.0884804	8.0990925	-1.0412074
C	3.8342969	7.0895183	0.8597149
H	2.5185889	5.5236284	1.6782350
H	1.2101604	7.2983637	-1.8641426
H	3.2233729	8.8594183	-1.8291504
H	4.5934048	7.0066723	1.6560595
Cl	-4.9857389	-0.0223094	2.1992134
N	-9.1034718	2.8459445	-0.0005353
C	-6.9282043	2.3040646	-0.8762843
C	-7.7109620	1.1310933	0.9496901
C	-8.8906700	1.8866300	0.9129378
C	-8.1037900	3.0743838	-0.8621579
H	-6.1425347	2.4688657	-1.6242107
H	-7.5192683	0.3783797	1.7275250
H	-9.6857579	1.7014613	1.6546353
H	-8.2261388	3.8955584	-1.5872741
Al	-0.2723464	-0.3689640	4.1812817
Cl	-1.8060830	-1.8909721	4.3802592
Cl	0.5248394	0.3072042	6.0424376
Cl	-1.1450195	1.2972948	3.0416480
Cl	1.2968947	-1.2065302	2.8826252
Al	-0.0562676	0.0482292	-3.6001653
Cl	-0.5404758	-1.9711424	-4.2026907
Cl	-0.1419958	0.0709377	-1.3833995
Cl	-1.4815742	1.4738976	-4.3710060
Cl	1.9721332	0.5847966	-4.1272817
Al	5.8631741	-5.7473582	0.6868167
Cl	7.5161407	-7.0040764	0.1672786
Cl	4.2603880	-6.7592158	1.7471999
Cl	5.0014348	-4.9351918	-1.1849134
Cl	6.4751093	-4.0700848	1.9383958
Al	-5.6707922	5.7463816	1.1800351
Cl	-7.1511901	7.2632347	0.8920823
Cl	-6.4290794	4.0079277	2.2462846
Cl	-3.9212086	6.4608611	2.2634458
Cl	-4.9785779	5.0556307	-0.8094352

$(AlCl_3)_2bipy_3$ (staggered, C_2)



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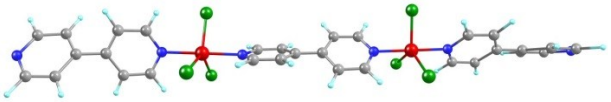
Cl	5.4916029	-1.8779964	-2.1481553
Cl	-5.8302850	-1.2461832	-0.0308999
Cl	5.8302850	1.2461832	-0.0308999
Cl	-5.6166772	2.1862200	1.6342320

E = -4731.117911367

Cl	5.6166772	-2.1862200	1.6342320
Al	5.6567823	-0.9359359	-0.1694105
Al	-5.6567823	0.9359359	-0.1694105
N	3.5071471	-0.6826437	-0.1262765
N	-3.5071471	0.6826437	-0.1262765
N	-14.7779054	2.6426517	0.4133635
N	14.7779054	-2.6426517	0.4133635
N	-7.7880504	1.2013012	-0.1941518
N	7.7880504	-1.2013012	-0.1941518
C	-10.5565535	1.7634849	0.0305938
C	-8.6456403	0.2807493	0.2997937
C	-8.2907696	2.3946117	-0.5886076
C	-9.6470640	2.7107507	-0.4919211
C	-10.0178177	0.5195749	0.4249872
H	-8.1895723	-0.6759556	0.5973266
H	-7.5641990	3.1038528	-1.0123184
H	-9.9943808	3.6899342	-0.8507136
H	-10.6579332	-0.2624130	0.8576506
C	-12.0055474	2.0640794	0.1596527
C	10.5565535	-1.7634849	0.0305938
C	8.6456403	-0.2807493	0.2997937
C	8.2907696	-2.3946117	-0.5886076
C	9.6470640	-2.7107507	-0.4919211
C	10.0178177	-0.5195749	0.4249872
H	8.1895723	0.6759556	0.5973266
H	7.5641990	-3.1038528	-1.0123184
H	9.9943808	-3.6899342	-0.8507136
H	10.6579332	0.2624130	0.8576506
C	12.0055474	-2.0640794	0.1596527
C	0.7291874	-0.1393884	-0.1202291
C	-0.7291874	0.1393884	-0.1202291
C	2.8896474	-0.2060093	-1.2316437
C	-2.8896474	0.2060093	-1.2316437
C	2.7622715	-0.8913391	0.9813531
C	-2.7622715	0.8913391	0.9813531
C	1.3883132	-0.6315768	1.0262197
C	-1.3883132	0.6315768	1.0262197
C	1.5216789	0.0722846	-1.2707368
C	-1.5216789	-0.0722846	-1.2707368
H	3.5295888	-0.0610640	-2.1145638
H	-3.5295888	0.0610640	-2.1145638
H	3.3086070	-1.2985947	1.8462063
H	-3.3086070	1.2985947	1.8462063
H	0.8339515	-0.8477918	1.9506860
H	-0.8339515	0.8477918	1.9506860
H	-1.0847200	-0.4768303	-2.1948337
H	1.0847200	0.4768303	-2.1948337
C	12.9876332	-1.0633474	-0.0104449
C	-12.9876332	1.0633474	-0.0104449

C	12.4642279	-3.3655746	0.4618264
C	-12.4642279	3.3655746	0.4618264
C	13.8444326	-3.5950056	0.5788447
C	-13.8444326	3.5950056	0.5788447
C	14.3430434	-1.4047402	0.1228251
C	-14.3430434	1.4047402	0.1228251
H	12.7045868	-0.0326072	-0.2719840
H	-12.7045868	0.0326072	-0.2719840
H	11.7548527	-4.1890549	0.6340631
H	-11.7548527	4.1890549	0.6340631
H	14.2136466	-4.6068110	0.8246782
H	-14.2136466	4.6068110	0.8246782
H	-15.1200554	0.6319604	-0.0174123
H	15.1200554	-0.6319604	-0.0174123

$(AlCl_3)_2bipy_3$ (eclipsed, C_2)



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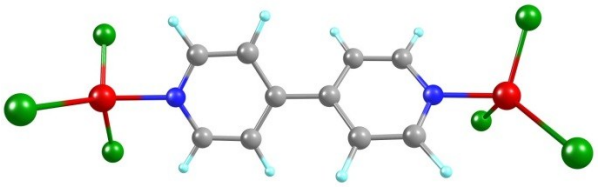
	X	Y	Z
Cl	5.9512080	0.1019620	-2.1335780
Al	5.7288233	-0.1438010	0.0369667
Cl	5.6269035	-2.1628553	0.8980987
Cl	5.5715951	1.5951629	1.3684909
N	7.8716415	-0.1677589	0.1729612
N	3.5706295	-0.1282949	-0.1011153
C	10.7033942	-0.2108621	0.0698662
C	8.5965705	0.9129751	0.5379126
C	8.5369119	-1.2729478	-0.2370517
C	9.9301200	-1.3328074	-0.3054927
C	9.9943920	0.9301592	0.5031946
H	8.0102082	1.7831850	0.8707187
H	7.9115355	-2.1400307	-0.4969311
H	10.4096312	-2.2688280	-0.6253369
H	10.5236899	1.8492765	0.7923701
C	12.1874926	-0.2318633	0.0119998
N	15.0280060	-0.2679132	-0.1023636
C	12.9737015	0.4606572	0.9593267
C	12.8770752	-0.9436156	-0.9944903
C	14.2810391	-0.9245099	-1.0061799
C	14.3730229	0.4061851	0.8581010
H	12.5040565	1.0144993	1.7860826
H	12.3287168	-1.4842777	-1.7806116
H	14.8308649	-1.4689067	-1.7947890
H	14.9980609	0.9358850	1.5992469
C	0.7420239	-0.0253858	-0.0978655
C	2.8896202	0.2420252	-1.2068611
C	2.8646255	-0.4487528	1.0079220
C	1.4696584	-0.4068357	1.0522576
C	1.4921437	0.3028989	-1.2467412
H	3.5117945	0.4899551	-2.0809614
H	3.4548838	-0.7666427	1.8798787
H	0.9548509	-0.7033718	1.9771631

H	0.9989629	0.6328965	-2.1721887
C	-0.7420239	0.0253858	-0.0978655
N	-3.5706295	0.1282949	-0.1011153
C	-1.4921437	-0.3028989	-1.2467412
C	-1.4696584	0.4068357	1.0522576
C	-2.8646255	0.4487528	1.0079220
C	-2.8896202	-0.2420252	-1.2068611
H	-0.9989629	-0.6328965	-2.1721887
H	-0.9548509	0.7033718	1.9771631
H	-3.4548838	0.7666427	1.8798787
H	-3.5117945	-0.4899551	-2.0809614
Cl	-5.9512080	-0.1019620	-2.1335780
Al	-5.7288233	0.1438010	0.0369667
Cl	-5.5715951	-1.5951629	1.3684909
Cl	-5.6269035	2.1628553	0.8980987
N	-7.8716415	0.1677589	0.1729612
C	-10.7033942	0.2108621	0.0698662
C	-8.5369119	1.2729478	-0.2370517
C	-8.5965705	-0.9129751	0.5379126
C	-9.9943920	-0.9301592	0.5031946
C	-9.9301200	1.3328074	-0.3054927
H	-7.9115355	2.1400307	-0.4969311
H	-8.0102082	-1.7831850	0.8707187
H	-10.5236899	-1.8492765	0.7923701
H	-10.4096312	2.2688280	-0.6253369
C	-12.1874926	0.2318633	0.0119998
N	-15.0280060	0.2679132	-0.1023636
C	-12.8770752	0.9436156	-0.9944903
C	-12.9737015	-0.4606572	0.9593267
C	-14.3730229	-0.4061851	0.8581010
C	-14.2810391	0.9245099	-1.0061799
H	-12.3287168	1.4842777	-1.7806116
H	-12.5040565	-1.0144993	1.7860826
H	-14.9980609	-0.9358850	1.5992469
H	-14.8308649	1.4689067	-1.7947890

$(AlCl_3)_2$bipy (C_2)

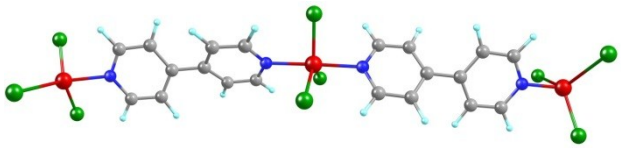


E = -3740.974352237

	X	Y	Z
C	0.6628286	-0.3350077	0.0023073
C	1.1588521	-0.9845606	-1.1500953
C	2.4077997	-1.6075257	-1.1090657
N	3.1746579	-1.6019532	0.0068827
C	2.7140688	-0.9928653	1.1248918
C	1.4743673	-0.3523269	1.1589004
H	0.5661670	-1.0400413	-2.0739049
H	2.8256804	-2.1497654	-1.9718974
H	3.3736738	-1.0448266	2.0053821
H	1.1597077	0.1498695	2.0843750
C	-0.6628286	0.3350077	0.0023073
C	-1.4743673	0.3523269	1.1589004

C	-2.7140688	0.9928653	1.1248918
N	-3.1746579	1.6019532	0.0068827
C	-2.4077997	1.6075257	-1.1090657
C	-1.1588521	0.9845606	-1.1500953
H	-1.1597077	-0.1498695	2.0843750
H	-3.3736738	1.0448266	2.0053821
H	-2.8256804	2.1497654	-1.9718974
H	-0.5661670	1.0400413	-2.0739049
Al	5.0389758	-2.4021428	-0.0156655
Cl	6.2450039	-0.7278635	-0.5553291
Cl	5.2425541	-3.0668200	2.0092725
Cl	4.8347471	-3.9151204	-1.5160538
Al	-5.0389758	2.4021428	-0.0156655
Cl	-6.2450039	0.7278635	-0.5553291
Cl	-5.2425541	3.0668200	2.0092725
Cl	-4.8347471	3.9151204	-1.5160538

$(AlCl_3)_3(bipy)_2$ (C_2)



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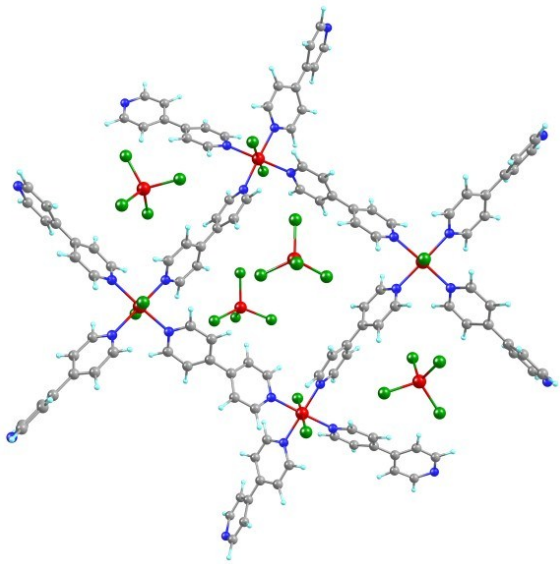
	X	Y	Z
C	4.8785182	-0.9326283	0.1488330
C	6.3454900	-1.1059453	0.0009211
N	9.1314685	-1.3926967	-0.2945156
C	7.2009595	-1.1739709	1.1240015
C	6.9440437	-1.2033306	-1.2753839
C	8.3282658	-1.3440438	-1.3839834
C	8.5761990	-1.3235971	0.9394233
H	6.7992900	-1.1409735	2.1464974
H	6.3402809	-1.1426048	-2.1916624
H	8.8387178	-1.4286112	-2.3563614
H	9.2766526	-1.4105543	1.7848165
Al	11.1446924	-1.4532155	-0.4999225
N	2.0889087	-0.5518250	0.3876103
C	3.9722860	-1.5521831	-0.7376711
C	4.3299871	-0.1306511	1.1737722
C	2.9447009	0.0348819	1.2547285
C	2.5986513	-1.3420161	-0.5825340
H	4.3227727	-2.2213304	-1.5365380
H	4.9741879	0.3972102	1.8913933
H	2.4829815	0.6534379	2.0392052
H	1.8568639	-1.8188635	-1.2418931
Al	0.0000000	0.0000000	0.4172705
Cl	11.6972708	0.6074909	-0.4417238
Cl	11.3724090	-2.3990187	-2.4082467
Cl	11.7127051	-2.5985134	1.2174134
N	-2.0889087	0.5518250	0.3876103
Cl	0.5747114	1.8128429	-0.6721659
Cl	0.0000000	0.0000000	2.6107015
Cl	-0.5747114	-1.8128429	-0.6721659
C	-4.8785182	0.9326283	0.1488330
C	-2.9447009	-0.0348819	1.2547285

C	-2.5986513	1.3420161	-0.5825340
C	-3.9722860	1.5521831	-0.7376711
C	-4.3299871	0.1306511	1.1737722
H	-2.4829815	-0.6534379	2.0392052
H	-1.8568639	1.8188635	-1.2418931
H	-4.3227727	2.2213304	-1.5365380
H	-4.9741879	-0.3972102	1.8913933
C	-6.3454900	1.1059453	0.0009211
N	-9.1314685	1.3926967	-0.2945156
C	-6.9440437	1.2033306	-1.2753839
C	-7.2009595	1.1739709	1.1240015
C	-8.5761990	1.3235971	0.9394233
C	-8.3282658	1.3440438	-1.3839834
H	-6.3402809	1.1426048	-2.1916624
H	-6.7992900	1.1409735	2.1464974
H	-9.2766526	1.4105543	1.7848165
H	-8.8387178	1.4286112	-2.3563614
Al	-11.1446924	1.4532155	-0.4999225
Cl	-11.6972708	-0.6074909	-0.4417238
Cl	-11.3724090	2.3990187	-2.4082467
Cl	-11.7127051	2.5985134	1.2174134

$[Al_4Cl_8bipy_{12}]^{4+}([AlCl_4]^-)_4$ (C_1)



E = -18924.48516218

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Cl	-7.4917009	0.5871413	-4.3099301
N	-8.8661083	-1.6870070	-2.6661112
N	-5.0418078	-1.2916427	-4.4289436
N	-7.7837194	-2.2444671	-5.4576136
N	-6.2040834	-0.8192040	-1.7831645
C	-5.0307366	0.0269415	0.6313406
C	-6.2498829	-1.6047908	-0.6761518
C	-5.5824474	0.3860356	-1.6930069
C	-4.9920318	0.8459409	-0.5135277
C	-5.6666831	-1.2278548	0.5306560
H	-6.7666203	-2.5686601	-0.7764710
H	-5.5573081	0.9989330	-2.6052897
H	-4.4703579	1.8167462	-0.5130309
H	-5.7658579	-1.8823007	1.4079370
C	-4.5047511	0.4572146	1.9483336
C	-2.4306123	-0.6713865	-5.2890729
C	-3.9623109	-1.6520960	-3.6939273
C	-4.8319827	-0.6566613	-5.6049597
C	-3.5524368	-0.3652840	-6.0850881
C	-2.6545251	-1.3322408	-4.0651426
H	-4.1661428	-2.2063748	-2.7669691
H	-5.7333323	-0.3328394	-6.1452588
H	-3.4398943	0.1644287	-7.0416561
H	-1.8275251	-1.5936111	-3.3893147

C	-1.0569555	-0.2721383	-5.7003695
N	-3.8352123	1.1083268	4.6068485
C	-3.6833552	-0.3900394	2.7181813
C	-4.8973584	1.6861690	2.5166978
C	-4.5448749	1.9721173	3.8352399
C	-3.3860674	-0.0381585	4.0339590
H	-3.2692445	-1.3199291	2.3030909
H	-5.5220826	2.3934739	1.9551024
H	-4.8396314	2.9161606	4.3155629
H	-2.7959637	-0.7164890	4.6644953
Al	-3.6146782	1.4458863	6.6431417
N	1.5687235	0.4656063	-6.4176223
C	-0.3342283	0.6669165	-4.9382609
C	-0.4366663	-0.8084198	-6.8486981
C	0.8751398	-0.4371096	-7.1541059
C	0.9543357	1.0246840	-5.3447228
H	-0.7714569	1.1575267	-4.0543846
H	-0.9525867	-1.5458903	-7.4805845
H	1.4224117	-0.8983659	-7.9888254
H	1.5116464	1.7969758	-4.7946459
Al	3.5988486	0.8928270	-6.8125377
N	-3.3051426	1.7767276	8.7571617
N	-5.6864296	1.8157936	6.8673491
N	-1.4917851	1.0778720	6.4138343
Cl	-3.2937148	3.6922662	6.3265118
Cl	-4.0011142	-0.7476233	7.1118542
N	5.6425825	1.3001600	-7.1568552
Cl	3.2189065	3.1034038	-6.4252493
Cl	3.9556193	-1.3008408	-7.3198214
N	3.1456481	1.2432826	-8.8845363
N	4.0277573	0.5537319	-4.7872500
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C	4.6754920	1.4989338	-4.0633624
C	5.0425354	1.3038812	-2.7331403
C	4.0157007	-0.8765757	-2.8420573
H	3.2003177	-1.3609994	-4.8051249
H	4.8889544	2.4425761	-4.5857042
H	5.6240384	2.0772883	-2.2135731
H	3.7122150	-1.8298246	-2.3872744
C	5.1866658	-0.1681184	-0.7156028
N	6.2753671	-0.5625872	1.8525698
C	5.8483605	-1.3656999	-0.3830303
C	5.0528092	0.8099345	0.2904246
C	5.6063917	0.5780888	1.5466421
C	6.3774842	-1.5215230	0.8994469
H	6.0184690	-2.1484812	-1.1346247
H	4.5167104	1.7503747	0.1000800
H	5.5586865	1.3372579	2.3398316

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Al	7.1557895	-0.8023763	3.7309705
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C	0.6391628	1.7182736	5.4659980
C	0.3861706	-0.4452023	6.4887244
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C	3.6974414	0.9412058	5.8187489
C	2.8685438	-0.9845155	4.6190325
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C	4.9825349	0.6093374	5.3852244
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N	9.0317586	-1.1032874	2.8211277
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Cl	6.7830863	-3.0482019	3.7249434
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C	-7.7007827	-3.7699176	-7.3294194
C	-9.4508233	-2.1268352	-7.2024758
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C	-7.5002546	3.1812388	7.6929294
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H	-10.5731476	1.4403451	5.5273731
H	-9.7556416	3.7809912	9.1289352
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C	-2.6749288	2.4210146	12.9876798
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C	-2.8147924	1.3739037	13.9254534
C	-2.3224851	3.6919999	13.4939397
C	-2.1351156	3.8495392	14.8765656
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H	-3.0624678	0.3521088	13.6008319

H	-2.2231620	4.5603849	12.8255515
H	-1.8690009	4.8406973	15.2852864
H	-2.6941701	0.8284381	16.0283346
C	9.1573781	-1.3520387	8.2656310
C	7.4861010	-1.8946080	6.5816563
C	9.0978328	-0.3062939	6.0685849
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C	8.0143369	-2.0777164	7.8616915
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H	9.4741067	0.4158851	5.3289933
H	10.6002961	0.1349898	7.5496498
H	7.5187921	-2.7814293	8.5453924
C	9.7598928	-1.5303340	9.6108191
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C	10.3894508	-0.4609241	10.2857536
C	10.9390596	-0.6846256	11.5583625
C	10.3171239	-2.8916341	11.5435957
H	9.2811238	-3.6625754	9.7967848
H	10.4286898	0.5448326	9.8411436
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C	9.8111761	-2.1696823	3.1298362
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H	9.3934754	-2.8714965	3.8664079
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H	12.6948461	-3.9045331	0.8029351
H	14.9276172	-4.1750336	-0.2969728
H	15.5544199	-0.0606853	-0.4038581
C	2.5631463	1.7372764	-11.6183305
C	2.1861718	2.1293694	-9.2456326
C	3.8154276	0.5973511	-9.8690027
C	3.5654145	0.8216372	-11.2253679
C	1.8631055	2.3909720	-10.5793713
H	1.6879661	2.6560599	-8.4179263
H	4.5619560	-0.1380826	-9.5330702
H	4.1716442	0.2901906	-11.9725709

H	1.0513541	3.0982227	-10.7999802
C	2.2621196	2.0014411	-13.0484267
N	1.6878427	2.5102519	-15.7847643
C	1.8243670	3.2709304	-13.4873166
C	2.4010825	0.9963485	-14.0312754
C	2.1006926	1.3013388	-15.3685749
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H	1.7181756	4.1093850	-12.7826784
H	2.7120487	-0.0236193	-13.7593373
H	2.1969307	0.5211572	-16.1446865
H	1.2244748	4.4592455	-15.2081738
C	8.4034012	1.8842658	-7.4935847
C	6.6012291	0.4634859	-6.6845004
C	6.0471701	2.4292668	-7.7909609
C	7.3918308	2.7414150	-7.9897827
C	7.9675867	0.7242818	-6.8142196
H	6.2580190	-0.4501793	-6.1791265
H	5.2464784	3.1138608	-8.1064886
H	7.6455911	3.6824997	-8.4973809
H	8.6768982	0.0076241	-6.3754352
C	9.8447506	2.1963431	-7.6704213
N	12.6015714	2.8025007	-8.0098308
C	10.3022839	2.9807607	-8.7540136
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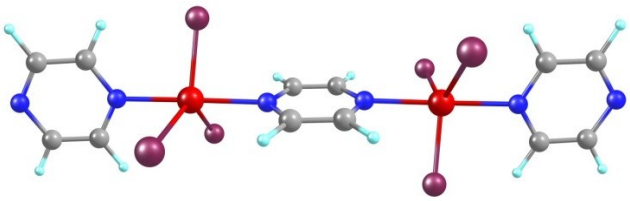
C	12.1660716	2.0555306	-6.9800447
C	11.6745879	3.2480230	-8.8748625
H	9.6057656	3.3613188	-9.5162690
H	10.5506435	1.1128196	-5.8858625
H	12.9332599	1.6930171	-6.2735320
H	12.0434720	3.8542199	-9.7219111
Al	0.3077866	-2.8394477	1.5548553
Cl	-1.1592582	-2.0131517	0.1826165
Cl	0.4779101	-4.9737160	1.3567486
Cl	-0.3233029	-2.3305875	3.6103020
Cl	2.2614688	-1.8951085	1.2350402
Al	9.0690443	-0.9924702	-2.6751346
Cl	7.3163860	-1.5599266	-3.8470989
Cl	9.3966006	-2.5402730	-1.1894691
Cl	8.6960144	0.9038002	-1.6527430
Cl	10.7625338	-0.7881260	-4.0173802
Al	-8.9218262	-1.0970127	2.6847402
Cl	-9.3436032	-2.7981685	1.3993571
Cl	-10.5176252	-0.8003432	4.1340144
Cl	-8.6767485	0.6971303	1.4728117
Cl	-7.0864253	-1.5156640	3.7965793
Al	-1.9449911	3.6988131	-2.2279265
Cl	-3.1310172	2.2627479	-3.4087063
Cl	-2.6569033	3.6494587	-0.1703121
Cl	-2.1569957	5.6579205	-3.0903956

Cl	0.1314889	3.0236190	-2.3009548

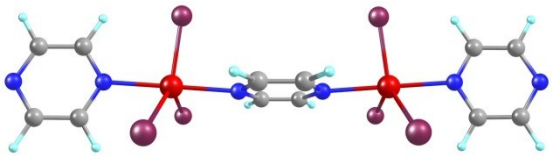
$(AlBr_3)_2pyz_3$ (staggered, C_i)



E = -16722.52057282

	X	Y	Z
Br	-3.7048386	0.6198733	-1.9858256
Al	-3.6102419	-0.1540890	0.2367017
Br	-3.7209952	1.3707004	2.0257867
Br	-3.3119335	-2.4509437	0.6529687
N	-5.7789040	-0.2723568	0.3002957
N	-1.3979606	-0.0106088	0.1204323
N	1.3979606	0.0106088	-0.1204323
C	-0.7727557	-0.6646630	-0.8801295
C	-0.6225581	0.6547272	1.0013260
C	0.7727557	0.6646630	0.8801295
C	0.6225581	-0.6547272	-1.0013260
H	-1.4026644	-1.2034495	-1.6028685
H	-1.1422745	1.1878307	1.8125833
H	1.4026644	1.2034495	1.6028685
H	1.1422745	-1.1878307	-1.8125833
N	-8.5913208	-0.2349456	0.4567658
C	-6.4705833	-1.3351875	0.7614124
C	-6.4917664	0.8118058	-0.0818489
C	-7.8915513	0.8175026	0.0007061
C	-7.8742080	-1.3027890	0.8342403
H	-5.8789945	-2.2132726	1.0647456
H	-5.9255534	1.6739503	-0.4648676
H	-8.4589779	1.7087354	-0.3166315
H	-8.4253954	-2.1804967	1.2126481
Br	3.7209952	-1.3707004	-2.0257867
Al	3.6102419	0.1540890	-0.2367017
Br	3.3119335	2.4509437	-0.6529687
Br	3.7048386	-0.6198733	1.9858256
N	5.7789040	0.2723568	-0.3002957
N	8.5913208	0.2349456	-0.4567658
C	6.4917664	-0.8118058	0.0818489
C	6.4705833	1.3351875	-0.7614124
C	7.8742080	1.3027890	-0.8342403
C	7.8915513	-0.8175026	-0.0007061
H	5.9255534	-1.6739503	0.4648676
H	5.8789945	2.2132726	-1.0647456
H	8.4253954	2.1804967	-1.2126481
H	8.4589779	-1.7087354	0.3166315

$(AlBr_3)_2pyz_3$ (eclipsed, C_s)



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Al	0.0257280	0.0648157	3.6161284
Br	0.8948143	2.2420452	3.8478663
Br	1.4963862	-1.7743487	3.6195498
N	-0.1041488	-0.0538360	5.7813545
N	0.1739200	0.1485594	1.4037448

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N	0.1739200	0.1485594	-1.4037448
C	0.0150920	-0.9944145	0.6985585
C	0.3289505	1.2867987	0.7018767
C	0.3289505	1.2867987	-0.7018767
C	0.0150920	-0.9944145	-0.6985585
H	-0.1002423	-1.9265332	1.2708333
H	0.4653889	2.2125257	1.2824729
H	0.4653889	2.2125257	-1.2824729
H	-0.1002423	-1.9265332	-1.2708333
N	-0.1034783	-0.1420264	8.5964293
C	1.0459913	0.0282120	6.4889131
C	-1.2515981	-0.1797563	6.4795251
C	-1.2364547	-0.2226374	7.8849842
C	1.0327838	-0.0166255	7.8900462
H	1.9811439	0.1278437	5.9176379
H	-2.1803179	-0.2473793	5.8909447
H	-2.1831369	-0.3265949	8.4420817
H	1.9787789	0.0518494	8.4533299
Br	1.4963862	-1.7743487	-3.6195498
Al	0.0257280	0.0648157	-3.6161284
Br	-2.2796009	-0.2784977	-3.2927311
Br	0.8948143	2.2420452	-3.8478663
N	-0.1041488	-0.0538360	-5.7813545
N	-0.1034783	-0.1420264	-8.5964293
C	1.0459913	0.0282120	-6.4889131
C	-1.2515981	-0.1797563	-6.4795251
C	-1.2364547	-0.2226374	-7.8849842
C	1.0327838	-0.0166255	-7.8900462
H	1.9811439	0.1278437	-5.9176379
H	-2.1803179	-0.2473793	-5.8909447
H	-2.1831369	-0.3265949	-8.4420817
H	1.9787789	0.0518494	-8.4533299

$[Al_4Br_8pyz_{12}]^{4+}([AlBr_4]^-)_4$ (C_1)

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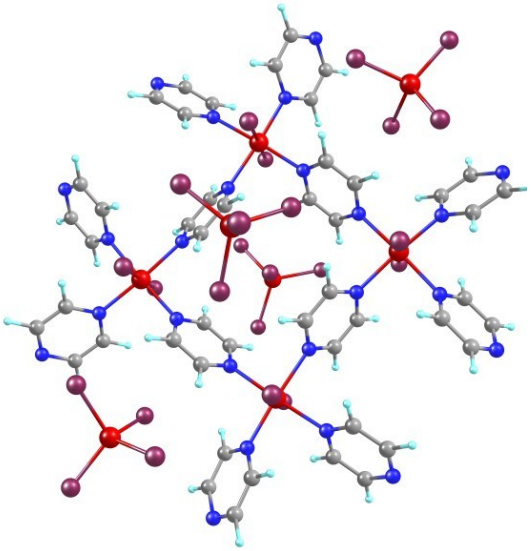
N	5.584801400	3.356050600	0.784906300
Al	3.405478400	3.640169900	0.771140700
N	1.257887900	3.810745500	0.769797200
N	3.233380500	1.439957600	0.583263400
N	3.715364800	5.726242200	0.992101400
Br	3.479581600	3.837808100	-1.625928500
N	3.307494000	-1.360383200	0.217829500
C	3.820724600	0.618214700	1.486239800
C	2.617406400	0.845766000	-0.463759900
C	2.654168000	-0.550965900	-0.646094700
C	3.857496700	-0.767755200	1.305022200
H	4.256079600	1.084681400	2.382008200
H	2.107381400	1.484911200	-1.203441600
H	2.175922600	-1.005264900	-1.529340400
H	4.321552200	-1.425355400	2.054687100



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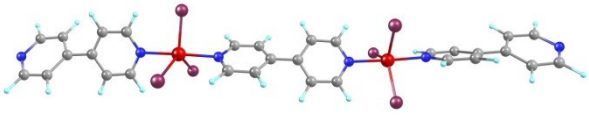
Al	3.599179200	-3.523281500	-0.165107800
N	8.389523600	3.067321500	0.756163700
C	6.217385700	2.710877200	-0.222197000
C	6.356701900	3.855006100	1.776941100
C	7.754406600	3.714424500	1.744960800
C	7.614584900	2.565480500	-0.217682600
H	5.589604000	2.346028000	-1.050640900
H	5.834147500	4.349177000	2.610080800
H	8.369835800	4.141896900	2.554524000
H	8.115355100	2.032939600	-1.043902900
N	-1.555934000	3.745956400	0.635099000
C	0.519088000	3.121348900	1.670455700
C	0.579882300	4.521150300	-0.161286400
C	-0.824306600	4.491605100	-0.226309400
C	-0.877131900	3.086337700	1.604765100
H	1.052601100	2.580996100	2.464664200
H	1.157181500	5.115380600	-0.886464000
H	-1.354581000	5.066387400	-1.001303000
H	-1.447802600	2.513747400	2.351581900
Al	-3.668463700	3.495569300	0.431216700
Br	3.422027900	3.419510100	3.209611900
N	4.037506000	-5.571307100	-0.482712200
N	5.762021000	-3.121078400	-0.065940100
N	1.463431700	-3.819473000	-0.228268000
Br	3.667588900	-3.093619400	-2.531706200
Br	3.628847100	-3.930932300	2.249489500
N	-1.354000500	-3.875664500	-0.360165100
C	0.694480800	-3.466998600	0.827271400
C	0.815473100	-4.268736600	-1.329728400
C	-0.588247100	-4.300450800	-1.394399400
C	-0.702439100	-3.491081900	0.762501800
H	1.197590100	-3.156652000	1.753558500
H	1.418190600	-4.594399300	-2.191468800
H	-1.091737000	-4.659448000	-2.305167000
H	-1.293884700	-3.191944600	1.640702400
Al	-3.481381500	-3.684782200	-0.493117300
N	-5.674317600	-3.394325200	-0.585546900
N	-3.790222600	-5.730513000	-0.880201400
Br	-3.375959700	-3.175234300	-2.854348200
Br	-3.737045600	-4.094171900	1.903788400
N	-5.838137100	3.125929700	0.239026600
N	-3.373970800	1.292579300	0.290361300
N	-4.085139100	5.557493600	0.569566000
Br	-3.529688000	3.614336600	-1.979804200
Br	-3.936307400	3.280224900	2.849806800
N	-3.301559000	-1.504916900	-0.071174500
C	-4.024697200	0.450803300	1.126018900
C	-2.613820800	0.723522200	-0.671541500
C	-2.576766400	-0.672766200	-0.851437600

C	-3.989566900	-0.936871900	0.945806200
H	-4.578101700	0.906287300	1.961428800
H	-2.040763700	1.376372100	-1.353237200
H	-1.975298600	-1.101250600	-1.672432400
H	-4.515667300	-1.617166200	1.632977000
N	4.331594700	8.441162700	1.433004600
C	3.086564700	6.447136600	1.947387800
C	4.603686900	6.387526800	0.209910100
C	4.916409000	7.731421000	0.455241600
C	3.391747000	7.805660800	2.144230100
H	2.359659100	5.924124400	2.582838100
H	5.053018700	5.822196100	-0.619534700
H	5.670185800	8.242777100	-0.166603700
H	2.853854700	8.378020700	2.917399000
N	-4.879653800	8.240209200	0.907362300
C	-3.599969000	6.315806300	1.578606100
C	-4.910900300	6.169217100	-0.315376400
C	-5.313965400	7.497156900	-0.122437900
C	-3.993058500	7.658295800	1.724422900
H	-2.921521700	5.835605200	2.296276700
H	-5.239040600	5.576817400	-1.182125300
H	-6.016481700	7.966501900	-0.831325000
H	-3.572944400	8.261634500	2.545652200
N	-8.618276100	2.742317900	-0.042633900
C	-6.715629600	3.625641500	1.138794400
C	-6.354346600	2.435368800	-0.803168300
C	-7.740133700	2.241435800	-0.924703800
C	-8.099334100	3.438218700	0.980361100
H	-6.290343100	4.158609300	2.002836000
H	-5.639755500	2.075345600	-1.559729200
H	-8.144501800	1.670035600	-1.777431900
H	-8.801210900	3.868125000	1.714747000
N	-8.474519300	-3.100649900	-0.757023300
C	-6.511938200	-4.152453900	0.157839000
C	-6.240478900	-2.490318700	-1.416876200
C	-7.636055900	-2.345918900	-1.483286700
C	-7.905692900	-4.005212900	0.054129300
H	-6.047707300	-4.864297800	0.857443100
H	-5.556232100	-1.912973400	-2.057960800
H	-8.081747500	-1.598735200	-2.161658800
H	-8.573538400	-4.644610800	0.655792100
N	-4.417538900	-8.453688400	-1.242809700
C	-3.241207200	-6.690653700	-0.102360700
C	-4.595543800	-6.144030200	-1.890040800
C	-4.915383800	-7.499425100	-2.044656800
C	-3.551207600	-8.047280600	-0.306318000
H	-2.575419500	-6.370595100	0.710064800
H	-4.975184900	-5.370085300	-2.572863500
H	-5.602875000	-7.813359200	-2.847890600

H	-3.078980300	-8.814243000	0.328836400
N	4.816489100	-8.267114900	-0.748215000
C	3.454054600	-6.549539800	0.244979000
C	4.962208100	-5.955414500	-1.396770200
C	5.356001200	-7.296241300	-1.501660300
C	3.840758300	-7.892678100	0.088673700
H	2.695825200	-6.253040800	0.981712800
H	5.375218600	-5.170027700	-2.046468000
H	6.138461500	-7.583979800	-2.223742700
H	3.338128700	-8.675707000	0.679431500
N	8.545566300	-2.672854500	-0.013668300
C	6.344498800	-2.205684800	-0.874260700
C	6.573367700	-3.809841200	0.768483500
C	7.960485300	-3.585139400	0.777002900
C	7.731122100	-1.985803000	-0.829535600
H	5.686948300	-1.679908600	-1.584373100
H	6.090293500	-4.529113100	1.447589600
H	8.608949700	-4.167707100	1.453024200
H	8.190760700	-1.233198600	-1.492311400
Br	-0.058281100	-0.264877800	1.687654700
Al	0.044984100	-0.584323600	4.079054200
Br	2.270749100	-0.313490200	4.685969600
Br	-1.325728100	1.055328900	4.973851200
Br	-0.711254600	-2.741290900	4.467959100
Br	0.277689600	0.876689200	-6.501826400
Al	0.939543200	0.580593000	-4.325423600
Br	3.264597600	0.603497100	-4.055523700
Br	0.031414100	2.253790500	-2.913249300
Br	0.116022900	-1.458611900	-3.446663100
Br	-2.011325100	7.842693800	-1.619311100
Al	-0.206549500	8.602657900	-0.330033300
Br	1.758993100	7.934967400	-1.409345500
Br	-0.293322700	10.861891300	0.092053000
Br	-0.294011800	7.421434700	1.752101400
Br	0.129417500	-7.628595600	-0.155023500
Al	0.246120300	-8.223689000	-2.471570800
Br	-1.592470400	-7.222445700	-3.529666100
Br	2.177511200	-7.230208600	-3.339245100
Br	0.237945200	-10.517298700	-2.649521200

$(AlBr_3)_2bipy_3$ (staggered, C_2)



E = -17415.25155822

	X	Y	Z
Br	-6.0048518	1.0218613	2.3368141
Al	-5.7446237	0.2553716	0.1142628
Br	-5.6758986	-2.0646796	-0.3662531
Br	-5.5143113	1.8433881	-1.6240417
N	-7.8999942	0.1738776	-0.0476987
N	-3.5692134	0.2035045	0.2554255
C	-10.7241654	-0.0827917	-0.1259395
C	-8.6422748	0.9097575	-0.9038774

C	-8.5474254	-0.6853710	0.7766649
C	-9.9337572	-0.8390365	0.7701220
C	-10.0362245	0.8104314	-0.9740946
H	-8.0769746	1.6002701	-1.5490521
H	-7.9154269	-1.2753126	1.4565383
H	-10.3913720	-1.5741263	1.4472383
H	-10.5802668	1.4547985	-1.6792085
C	-12.2017130	-0.2261004	-0.1718584
N	-15.0294798	-0.5108218	-0.2626889
C	-12.9200463	-0.0865851	-1.3801749
C	-12.9533230	-0.5125253	0.9894615
C	-14.3479851	-0.6398268	0.8882076
C	-14.3156156	-0.2401290	-1.3685394
H	-12.3983109	0.1100728	-2.3289420
H	-12.4637830	-0.6084708	1.9703745
H	-14.9462313	-0.8551638	1.7916242
H	-14.8863233	-0.1429055	-2.3094824
C	-0.7409744	0.0425532	0.2585514
C	-2.8575685	0.5100947	1.3611548
C	-2.8907559	-0.1820646	-0.8518814
C	-1.4987292	-0.2698732	-0.8931539
C	-1.4601051	0.4393540	1.4048199
H	-3.4499076	0.8258465	2.2344511
H	-3.5005224	-0.4335991	-1.7319236
H	-1.0128942	-0.6115821	-1.8180121
H	-0.9413823	0.7246926	2.3311117
C	0.7409744	-0.0425532	0.2585514
N	3.5692134	-0.2035045	0.2554255
C	1.4601051	-0.4393540	1.4048199
C	1.4987292	0.2698732	-0.8931539
C	2.8907559	0.1820646	-0.8518814
C	2.8575685	-0.5100947	1.3611548
H	0.9413823	-0.7246926	2.3311117
H	1.0128942	0.6115821	-1.8180121
H	3.5005224	0.4335991	-1.7319236
H	3.4499076	-0.8258465	2.2344511
Br	6.0048518	-1.0218613	2.3368141
Al	5.7446237	-0.2553716	0.1142628
Br	5.5143113	-1.8433881	-1.6240417
Br	5.6758986	2.0646796	-0.3662531
N	7.8999942	-0.1738776	-0.0476987
C	10.7241654	0.0827917	-0.1259395
C	8.5474254	0.6853710	0.7766649
C	8.6422748	-0.9097575	-0.9038774
C	10.0362245	-0.8104314	-0.9740946
C	9.9337572	0.8390365	0.7701220
H	7.9154269	1.2753126	1.4565383
H	8.0769746	-1.6002701	-1.5490521
H	10.5802668	-1.4547985	-1.6792085

H	10.3913720	1.5741263	1.4472383
C	12.2017130	0.2261004	-0.1718584
N	15.0294798	0.5108218	-0.2626889
C	12.9533230	0.5125253	0.9894615
C	12.9200463	0.0865851	-1.3801749
C	14.3156156	0.2401290	-1.3685394
C	14.3479851	0.6398268	0.8882076
H	12.4637830	0.6084708	1.9703745
H	12.3983109	-0.1100728	-2.3289420
H	14.8863233	0.1429055	-2.3094824
H	14.9462313	0.8551638	1.7916242

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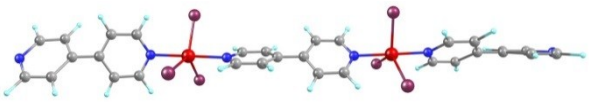

E = -17415.25159002

	X	Y	Z
Br	6.0511675	0.3741764	-2.2971679
Al	5.7525941	-0.0962207	0.0035743
Br	5.6389495	-2.3403345	0.7468411
Br	5.5269817	1.6464664	1.5901579
N	7.9127021	-0.1341644	0.1630944
N	3.5748400	-0.0833055	-0.1614173
C	10.7489394	-0.2079201	0.1002636
C	8.6479899	0.8607446	0.7074391
C	8.5732598	-1.1678638	-0.4122429
C	9.9657846	-1.2408077	-0.4638189
C	10.0466546	0.8597812	0.6984399
H	8.0734696	1.6820454	1.1633599
H	7.9462108	-1.9687077	-0.8315810
H	10.4359137	-2.1208200	-0.9248920
H	10.5807867	1.7137895	1.1385829
C	12.2333086	-0.2439550	0.0623173
N	15.0752278	-0.3094969	-0.0143662
C	13.0135847	0.3063419	1.1033345
C	12.9302376	-0.8282975	-1.0185542
C	14.3343016	-0.8304019	-1.0070472
C	14.4135212	0.2440361	1.0159512
H	12.5392186	0.7552579	1.9888609
H	12.3888111	-1.2527036	-1.8773500
H	14.8892261	-1.2760108	-1.8520833
H	15.0332356	0.6633152	1.8287849
C	0.7420341	-0.0182302	-0.1635628
C	2.8887696	0.2765550	-1.2675578
C	2.8681030	-0.4135445	0.9460500
C	1.4731359	-0.3914968	0.9872500
C	1.4902979	0.3183450	-1.3105136
H	3.5036102	0.5399092	-2.1426994
H	3.4567899	-0.7136815	1.8253370
H	0.9619177	-0.6933376	1.9123393
H	0.9961302	0.6434935	-2.2371238
C	-0.7420341	0.0182302	-0.1635628
N	-3.5748400	0.0833055	-0.1614173

C	-1.4902979	-0.3183450	-1.3105136
C	-1.4731359	0.3914968	0.9872500
C	-2.8681030	0.4135445	0.9460500
C	-2.8887696	-0.2765550	-1.2675578
H	-0.9961302	-0.6434935	-2.2371238
H	-0.9619177	0.6933376	1.9123393
H	-3.4567899	0.7136815	1.8253370
H	-3.5036102	-0.5399092	-2.1426994
Br	-6.0511675	-0.3741764	-2.2971679
Al	-5.7525941	0.0962207	0.0035743
Br	-5.5269817	-1.6464664	1.5901579
Br	-5.6389495	2.3403345	0.7468411
N	-7.9127021	0.1341644	0.1630944
C	-10.7489394	0.2079201	0.1002636
C	-8.5732598	1.1678638	-0.4122429
C	-8.6479899	-0.8607446	0.7074391
C	-10.0466546	-0.8597812	0.6984399
C	-9.9657846	1.2408077	-0.4638189
H	-7.9462108	1.9687077	-0.8315810
H	-8.0734696	-1.6820454	1.1633599
H	-10.5807867	-1.7137895	1.1385829
H	-10.4359137	2.1208200	-0.9248920
C	-12.2333086	0.2439550	0.0623173
N	-15.0752278	0.3094969	-0.0143662
C	-12.9302376	0.8282975	-1.0185542
C	-13.0135847	-0.3063419	1.1033345
C	-14.4135212	-0.2440361	1.0159512
C	-14.3343016	0.8304019	-1.0070472
H	-12.3888111	1.2527036	-1.8773500
H	-12.5392186	-0.7552579	1.9888609
H	-15.0332356	-0.6633152	1.8287849
H	-14.8892261	1.2760108	-1.8520833

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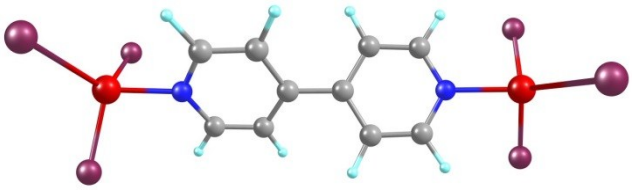

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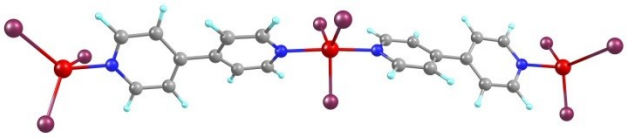
C	1.1549005	-0.9920515	-1.1369719
C	2.4044067	-1.6142006	-1.0989200
N	3.1798654	-1.6039086	0.0122934
C	2.7254321	-0.9795214	1.1255550
C	1.4839297	-0.3413687	1.1631035
H	0.5580355	-1.0541647	-2.0577069
H	2.8123470	-2.1597227	-1.9648079
H	3.3913861	-1.0144871	2.0025138
H	1.1761561	0.1686463	2.0866781
C	-0.6635248	0.3342320	0.0128940
C	-1.4839297	0.3413687	1.1631035
C	-2.7254321	0.9795214	1.1255550
N	-3.1798654	1.6039086	0.0122934
C	-2.4044067	1.6142006	-1.0989200

C	-1.1549005	0.9920515	-1.1369719
H	-1.1761561	-0.1686463	2.0866781
H	-3.3913861	1.0144871	2.0025138
H	-2.8123470	2.1597227	-1.9648079
H	-0.5580355	1.0541647	-2.0577069
Al	5.0526066	-2.4204604	-0.0272498
Br	6.3223991	-0.6457637	-0.7467005
Br	5.3727252	-3.0411111	2.1675219
Br	4.8190366	-4.1430603	-1.5382028
Al	-5.0526066	2.4204604	-0.0272498
Br	-6.3223991	0.6457637	-0.7467005
Br	-5.3727252	3.0411111	2.1675219
Br	-4.8190366	4.1430603	-1.5382028

$(AlBr_3)_3(bipy)_2$ (C_1)



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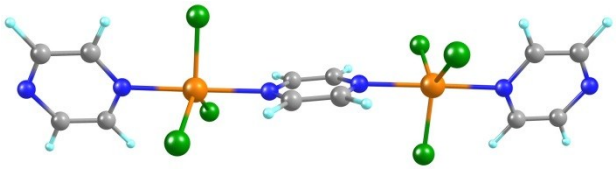
	X	Y	Z
C	4.9991091	0.0899796	-0.1220502
C	6.4781752	-0.0390665	-0.0987061
N	9.2869772	-0.2944011	-0.0642299
C	7.1079638	-1.1823848	0.4441535
C	7.3161532	0.9696220	-0.6244043
C	8.7026481	0.8100915	-0.5886670
C	8.5001153	-1.2769029	0.4391774
H	6.5186693	-2.0195558	0.8438543
H	6.8972617	1.8953449	-1.0431230
H	9.3905481	1.5707569	-0.9914126
H	9.0249642	-2.1640011	0.8275172
Al	11.3117168	-0.4472537	0.0844436
N	2.1781086	0.3015874	-0.1847506
C	4.3305469	0.7164723	-1.1937798
C	4.1978699	-0.4172186	0.9257962
C	2.8094967	-0.2881854	0.8582691
C	2.9326353	0.7967433	-1.1889045
H	4.8827098	1.1150946	-2.0568575
H	4.6473438	-0.8915144	1.8097150
H	2.1649266	-0.6748614	1.6613843
H	2.3761707	1.2612350	-2.0183093
Al	0.0000139	0.4105270	-0.1030081
Br	12.0669384	0.9499106	-1.5854415
Br	11.6761838	-2.6968612	-0.2538579
Br	11.6843447	0.2868832	2.2311097
N	-2.1787965	0.3855402	0.0186952
Br	0.2303250	1.9024383	1.7092148
Br	-0.0508817	-1.9293727	0.2451698
Br	-0.1858643	1.2759522	-2.2902592
C	-4.9982295	0.1550377	0.0783460
C	-2.8369932	-0.3520270	-0.9072406
C	-2.9052574	1.0133836	0.9677234
C	-4.3016088	0.9271083	1.0305591
C	-4.2254620	-0.4928640	-0.9120211

H	-2.2153123	-0.8409564	-1.6716487
H	-2.3263509	1.5978645	1.7003701
H	-4.8292970	1.4407992	1.8467673
H	-4.6981651	-1.0873501	-1.7065641
C	-6.4764876	0.0210612	0.1151163
N	-9.2845178	-0.2403370	0.1831493
C	-7.3059023	1.0857968	0.5342178
C	-7.1146875	-1.1816153	-0.2639956
C	-8.5061583	-1.2764151	-0.2139536
C	-8.6916790	0.9208159	0.5544696
H	-6.8813850	2.0570956	0.8240984
H	-6.5322995	-2.0614713	-0.5710419
H	-9.0389117	-2.2037233	-0.4786264
H	-9.3706740	1.7244854	0.8808827
Al	-11.3139257	-0.3822378	0.1008756
Br	-11.7542712	0.3633644	-2.0288455
Br	-11.9966255	1.0237243	1.7937925
Br	-11.6921723	-2.6281388	0.4528308

$(GaCl_3)_2pyz_3$ (staggered, C_i)

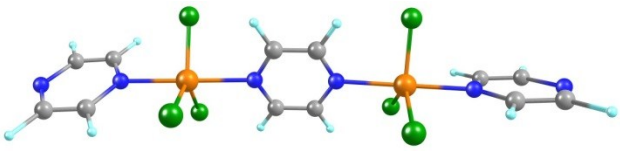


E = -7403.285060119

	X	Y	Z
Cl	-0.1292485	3.6744369	-2.3427035
Ga	-0.3615898	3.6487025	-0.1331524
Cl	1.4362513	3.6579047	1.1731585
Cl	-2.3968222	3.5001303	0.7563130
N	-0.4915066	5.8716560	-0.1374409
N	-0.2086073	1.3716714	-0.1066169
N	-0.6623623	8.6625925	-0.3578260
C	-1.6273932	6.4665146	-0.5524777
C	0.5580166	6.6563689	0.1728998
C	0.4586211	8.0537651	0.0584144
C	-1.6994910	7.8646327	-0.6601200
H	-2.4798768	5.8080879	-0.7801878
H	1.4668822	6.1417176	0.5235127
H	1.3203900	8.6930097	0.3161245
H	-2.6312630	8.3472587	-1.0010881
N	0.2086073	-1.3716714	0.1066169
C	0.4799570	0.7030973	-1.0497095
C	-0.6913809	0.6786214	0.9409600
C	-0.4799570	-0.7030973	1.0497095
C	0.6913809	-0.6786214	-0.9409600
H	0.8494326	1.2941798	-1.9024331
H	-1.2667051	1.2448842	1.6895729
H	-0.8494326	-1.2941798	1.9024331
H	1.2667051	-1.2448842	-1.6895729
Cl	0.1292485	-3.6744369	2.3427035
Ga	0.3615898	-3.6487025	0.1331524
Cl	-1.4362513	-3.6579047	-1.1731585
Cl	2.3968222	-3.5001303	-0.7563130
N	0.4915066	-5.8716560	0.1374409

N	0.6623623	-8.6625925	0.3578260
C	1.6273932	-6.4665146	0.5524777
C	-0.5580166	-6.6563689	-0.1728998
C	-0.4586211	-8.0537651	-0.0584144
C	1.6994910	-7.8646327	0.6601200
H	2.4798768	-5.8080879	0.7801878
H	-1.4668822	-6.1417176	-0.5235127
H	-1.3203900	-8.6930097	-0.3161245
H	2.6312630	-8.3472587	1.0010881

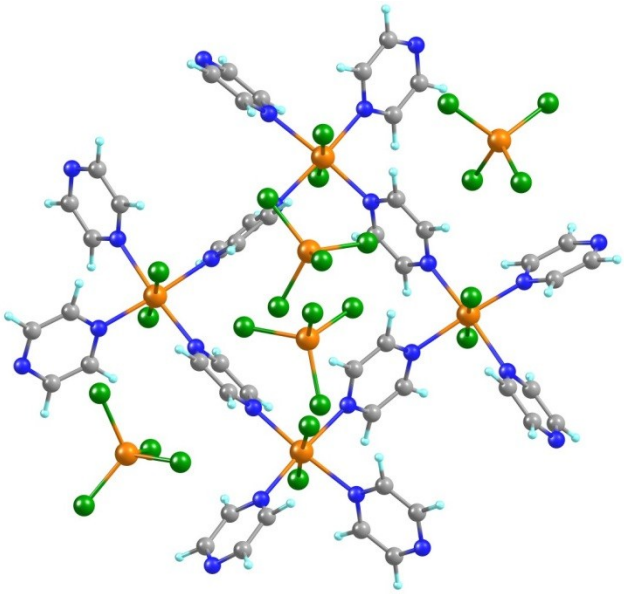
$(GaCl_3)_2pyz_3$ (eclipsed, C_2)



E = -7403.284989264

	X	Y	Z
Cl	3.4304906	-0.2669521	2.1582033
Ga	3.6754870	-0.0618568	-0.0385468
Cl	3.8106970	1.9581361	-0.9545795
Cl	3.6931625	-1.8711639	-1.3354239
N	5.8998152	-0.1085321	0.0957756
N	1.3925752	-0.0126368	-0.1934724
N	-1.3925752	0.0126368	-0.1934724
C	0.6902124	-1.1606498	-0.1935749
C	0.7120420	1.1483640	-0.1939269
C	-0.6902124	1.1606498	-0.1935749
C	-0.7120420	-1.1483640	-0.1939269
H	1.2678629	-2.0975369	-0.2197543
H	1.3119426	2.0718833	-0.2181907
H	-1.2678629	2.0975369	-0.2197543
H	-1.3119426	-2.0718833	-0.2181907
N	8.7002750	0.0435270	0.1409147
C	6.6263805	-0.3631084	-1.0103472
C	6.5575919	0.2161362	1.2250970
C	7.9613392	0.2887671	1.2338806
C	8.0276777	-0.2822486	-0.9749033
H	6.0695018	-0.6479341	-1.9164560
H	5.9376596	0.4027615	2.1166797
H	8.4962694	0.5538240	2.1618723
H	8.6183246	-0.4910059	-1.8832475
Cl	-3.8106970	-1.9581361	-0.9545795
Ga	-3.6754870	0.0618568	-0.0385468
Cl	-3.4304906	0.2669521	2.1582033
Cl	-3.6931625	1.8711639	-1.3354239
N	-5.8998152	0.1085321	0.0957756
N	-8.7002750	-0.0435270	0.1409147
C	-6.6263805	0.3631084	-1.0103472
C	-6.5575919	-0.2161362	1.2250970
C	-7.9613392	-0.2887671	1.2338806
C	-8.0276777	0.2822486	-0.9749033
H	-6.0695018	0.6479341	-1.9164560
H	-5.9376596	-0.4027615	2.1166797
H	-8.4962694	-0.5538240	2.1618723
H	-8.6183246	0.4910059	-1.8832475

$[Ga_4Cl_8pyz_{12}]^{4+}([GaCl_4]^-)_4$ (C_1)



E = -29613.12263048

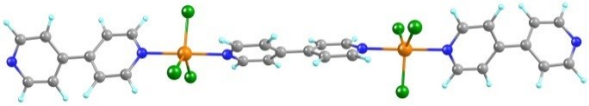
	X	Y	Z
N	-6.8445105	1.3529023	0.0415189
Ga	-5.0936513	0.0837118	-0.0146251
N	-3.3485567	-1.3774339	-0.1195935
N	-3.6697256	1.7372685	-0.0311411
N	-6.4691678	-1.7575238	-0.0209944
Cl	-5.2286636	0.0694894	-2.3195004
N	-1.6947837	3.7121315	-0.0620943
C	-3.4403053	2.5057487	1.0542247
C	-2.9460252	1.9837219	-1.1425462
C	-1.9568206	2.9703185	-1.1579334
C	-2.4482591	3.5017383	1.0374938
H	-4.0436760	2.3219587	1.9539249
H	-3.1471472	1.3867730	-2.0432452
H	-1.3700799	3.1537343	-2.0692392
H	-2.2555840	4.1239310	1.9225557
Ga	-0.0325521	5.1132785	-0.0894144
N	-1.3691543	-3.3592639	-0.1679613
C	-2.5717858	-1.6141213	0.9571826
C	-3.0857935	-2.0782298	-1.2430075
C	-2.0967733	-3.0698337	-1.2679573
C	-1.5774245	-2.6089517	0.9338433
H	-2.7669251	-1.0496447	1.8830655
H	-3.6846458	-1.8374393	-2.1341105
H	-1.8746153	-3.6401426	-2.1820937
H	-0.9780357	-2.8163640	1.8340531
Ga	0.0678207	-5.1197254	-0.1525497
N	1.8229851	6.4887122	-0.1517450
N	-1.2735596	6.8730797	-0.0118927
N	1.3789621	3.3463846	-0.2068831
Cl	-0.0376160	5.2223688	-2.3940100
Cl	0.1834878	5.0737622	2.1816648
N	1.3123776	-6.8970112	-0.1769536
N	1.7217078	-3.6985654	-0.1962380
N	-1.8077264	-6.4474889	-0.1182557
Cl	0.0033528	-5.2130669	-2.4482981
Cl	0.0442382	-5.1418757	2.1287407
N	3.6807864	-1.7151047	-0.1771936
C	2.5910966	-3.5955150	0.8271542
C	1.8527373	-2.8413974	-1.2320599
C	2.8374820	-1.8478928	-1.2242223
C	3.5760469	-2.5927440	0.8392366
H	2.4967481	-4.3078386	1.6590892
H	1.1596611	-2.9450039	-2.0816593
H	2.9435273	-1.1469127	-2.0673939
H	4.2775901	-2.5008561	1.6805766
Ga	5.0993319	-0.0673146	-0.1218908
N	3.3432367	1.3594083	-0.2204714

C	1.4633952	2.4478111	0.7958532
C	2.2114213	3.1957101	-1.2569357
C	3.1957439	2.1990634	-1.2655243
C	2.4519838	1.4484149	0.7880733
H	0.7572325	2.5245433	1.6404942
H	2.0750087	3.8844128	-2.1040634
H	3.8765716	2.0604270	-2.1181806
H	2.5251511	0.7286755	1.6201640
N	6.4578185	1.7937817	-0.0865021
N	6.8706641	-1.3006755	-0.0432975
Cl	5.2527069	-0.0315806	-2.4131058
Cl	5.0095071	0.0415063	2.1582841
N	8.1591663	4.0333109	-0.0220060
C	6.4617762	2.6392594	0.9653786
C	7.3019357	2.0605420	-1.1049850
C	8.1518632	3.1794589	-1.0574303
C	7.3120225	3.7581884	0.9819638
H	5.7922899	2.3837658	1.8022704
H	7.2680107	1.3725863	-1.9644911
H	8.8450247	3.3831223	-1.8914056
H	7.3048494	4.4452146	1.8454867
N	9.2669888	-2.7617572	-0.0433408
C	7.7973249	-1.1221677	0.9234521
C	7.1057607	-2.2506852	-0.9717294
C	8.3034938	-2.9876849	-0.9464954
C	8.9992198	-1.8444541	0.8978856
H	7.5545502	-0.4008264	1.7174874
H	6.3407705	-2.4121611	-1.7424772
H	8.4740580	-3.7807297	-1.6928542
H	9.7658964	-1.6656076	1.6705507
N	2.7328891	-9.3115398	-0.3532625
C	1.1303056	-7.8820270	0.7290577
C	2.2510581	-7.0838341	-1.1269407
C	2.9656424	-8.2930988	-1.1914545
C	1.8329840	-9.0906821	0.6166699
H	0.4191876	-7.6820575	1.5439626
H	2.4173362	-6.2726189	-1.8477750
H	3.7419431	-8.4280509	-1.9626467
H	1.6499651	-9.9036735	1.3395268
N	-4.1066041	-8.0683483	-0.0682330
C	-2.6231494	-6.4720694	0.9572090
C	-2.1339092	-7.2313780	-1.1671608
C	-3.2819882	-8.0417905	-1.1267200
C	-3.7717929	-7.2817297	0.9664924
H	-2.3230236	-5.8517628	1.8169503
H	-1.4697112	-7.1805858	-2.0441613
H	-3.5346787	-8.6854947	-1.9864889
H	-4.4336945	-7.2909799	1.8493234
N	-8.1842547	-3.9873430	0.0004575

C	-6.4731806	-2.6270931	1.0111701
C	-7.3193915	-1.9960912	-1.0413220
C	-8.1764387	-3.1100002	-1.0149770
C	-7.3299625	-3.7411583	1.0057793
H	-5.7995577	-2.3965344	1.8518860
H	-7.2856954	-1.2905539	-1.8859943
H	-8.8753925	-3.2894717	-1.8497245
H	-7.3219173	-4.4482646	1.8528418
N	-2.7970483	9.2290402	0.0122046
C	-2.2575463	7.0735722	-0.9122386
C	-1.0865843	7.8152483	0.9382415
C	-1.8414472	8.9970413	0.9245971
C	-3.0241279	8.2517442	-0.8754177
H	-2.4170588	6.2997568	-1.6743365
H	-0.3335935	7.5996741	1.7102718
H	-1.6588925	9.7763751	1.6834630
H	-3.8414391	8.3949471	-1.6011554
N	4.0467864	8.2114671	-0.1963610
C	2.7273881	6.4900317	0.8495483
C	2.0232572	7.3465277	-1.1737764
C	3.1343542	8.2077176	-1.1804128
C	3.8384090	7.3498911	0.8111271
H	2.5254300	5.8114044	1.6934137
H	1.2900668	7.3143832	-1.9946451
H	3.2824875	8.9129088	-2.0161049
H	4.5752511	7.3388999	1.6325262
Cl	-5.0619204	-0.0431818	2.2606823
N	-9.1747258	2.9173751	0.0501127
C	-7.0248555	2.3372529	-0.8624028
C	-7.7950251	1.1849132	0.9866163
C	-8.9635534	1.9599973	0.9656225
C	-8.1896254	3.1243750	-0.8336313
H	-6.2448090	2.4832172	-1.6208370
H	-7.5974364	0.4314104	1.7627854
H	-9.7493843	1.7927686	1.7213727
H	-8.3146751	3.9423176	-1.5620448
Ga	-0.2712444	-0.3662257	4.2596079
Cl	-1.9545886	-1.8142111	4.3772146
Cl	0.7037908	-0.0212711	6.1810978
Cl	-1.0306084	1.5402710	3.3553308
Cl	1.1803779	-1.2020671	2.7455665
Ga	-0.0418031	0.0655661	-3.5618304
Cl	-0.5160759	-2.0037261	-4.1836547
Cl	-0.1359837	0.0871619	-1.2956008
Cl	-1.5063486	1.5119141	-4.3582187
Cl	2.0333392	0.6154384	-4.0971566
Ga	5.8853685	-5.7836601	0.6895095
Cl	7.5794803	-7.0557633	0.1465379
Cl	4.2442662	-6.8168373	1.7714875

Cl	5.0018727	-4.9431290	-1.2207849
Cl	6.5018519	-4.0746016	1.9827625
Ga	-5.6592658	5.7508627	1.1991065
Cl	-7.1828270	7.2885003	0.8971815
Cl	-6.4058845	3.9730392	2.3085347
Cl	-3.8677364	6.4891728	2.2951575
Cl	-4.9564504	5.0320960	-0.8352051

$(GaCl_3)_2bipy_3$ (staggered, C_2)



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Cl	-5.9239827	-1.2869569	0.0455516
Cl	5.9239827	1.2869569	0.0455516
Cl	-5.6769456	2.2042024	1.7165345
Cl	5.6769456	-2.2042024	1.7165345
Ga	5.7239677	-0.9303204	-0.1174016
Ga	-5.7239677	0.9303204	-0.1174016
N	3.5019631	-0.6634311	-0.0683949
N	-3.5019631	0.6634311	-0.0683949
N	-14.9121524	2.6727070	0.3003847
N	14.9121524	-2.6727070	0.3003847
N	-7.9233788	1.2196968	-0.1711421
N	7.9233788	-1.2196968	-0.1711421
C	-10.6846566	1.7866096	0.0057151
C	-8.7811134	0.3050416	0.3251875
C	-8.4097209	2.4077915	-0.5886900
C	-9.7678571	2.7274618	-0.5160765
C	-10.1553670	0.5467766	0.4271108
H	-8.3260240	-0.6472694	0.6407416
H	-7.6719595	3.1062215	-1.0128001
H	-10.1109126	3.7015266	-0.8927907
H	-10.8048785	-0.2269607	0.8608496
C	-12.1358478	2.0895397	0.1056427
C	10.6846566	-1.7866096	0.0057151
C	8.7811134	-0.3050416	0.3251875
C	8.4097209	-2.4077915	-0.5886900
C	9.7678571	-2.7274618	-0.5160765
C	10.1553670	-0.5467766	0.4271108
H	8.3260240	0.6472694	0.6407416
H	7.6719595	-3.1062215	-1.0128001
H	10.1109126	-3.7015266	-0.8927907
H	10.8048785	0.2269607	0.8608496
C	12.1358478	-2.0895397	0.1056427
C	0.7303629	-0.1351885	-0.0562334
C	-0.7303629	0.1351885	-0.0562334
C	2.8884783	-0.1891901	-1.1725575
C	-2.8884783	0.1891901	-1.1725575
C	2.7683372	-0.8781694	1.0418469
C	-2.7683372	0.8781694	1.0418469

C	1.3921865	-0.6263249	1.0899673
C	-1.3921865	0.6263249	1.0899673
C	1.5183101	0.0837050	-1.2087024
C	-1.5183101	-0.0837050	-1.2087024
H	3.5298767	-0.0439357	-2.0552139
H	-3.5298767	0.0439357	-2.0552139
H	3.3228243	-1.2845275	1.9029544
H	-3.3228243	1.2845275	1.9029544
H	0.8383123	-0.8465023	2.0139070
H	-0.8383123	0.8465023	2.0139070
H	-1.0756548	-0.4879851	-2.1302890
H	1.0756548	0.4879851	-2.1302890
C	13.1154286	-1.0880684	-0.0738586
C	-13.1154286	1.0880684	-0.0738586
C	12.5990562	-3.3940198	0.3871217
C	-12.5990562	3.3940198	0.3871217
C	13.9810515	-3.6257038	0.4752285
C	-13.9810515	3.6257038	0.4752285
C	14.4728756	-1.4317841	0.0299229
C	-14.4728756	1.4317841	0.0299229
H	12.8283713	-0.0548800	-0.3210445
H	-12.8283713	0.0548800	-0.3210445
H	11.8922378	-4.2185719	0.5646366
H	-11.8922378	4.2185719	0.5646366
H	14.3538650	-4.6399545	0.7049745
H	-14.3538650	4.6399545	0.7049745
H	-15.2477715	0.6582474	-0.1179102
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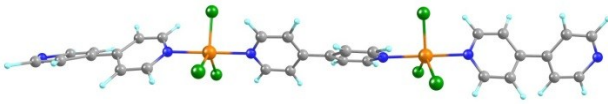
$(GaCl_3)_2bipy_3$ (eclipsed, C_2)



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Cl	5.9884930	-0.0088923	-2.1175979
Ga	5.7976814	-0.1969748	0.1004939
Cl	5.6985012	-2.2236312	1.0402257
Cl	5.6666308	1.6193668	1.3929773
N	8.0153170	-0.2150863	0.2159596
N	3.5594988	-0.1792600	-0.0212937
C	10.8344519	-0.2230991	0.0414946
C	8.7219809	0.9056432	0.4678389
C	8.6804786	-1.3426414	-0.1124310
C	10.0737807	-1.3872264	-0.2121511
C	10.1183342	0.9419512	0.3942380
H	8.1250359	1.7902470	0.7407780
H	8.0580790	-2.2358228	-0.2773298
H	10.5636788	-2.3394769	-0.4610277
H	10.6405880	1.8900650	0.5871007
C	12.3167464	-0.2242536	-0.0598036
N	15.1528589	-0.2196439	-0.2620018
C	13.1173842	0.5604192	0.7995387
C	12.9898002	-1.0073145	-1.0236416

C	14.3920315	-0.9647273	-1.0817912
C	14.5138243	0.5226557	0.6582054
H	12.6620937	1.1745947	1.5910593
H	12.4286957	-1.6222869	-1.7433137
H	14.9285795	-1.5649486	-1.8383095
H	15.1501348	1.1252810	1.3309081
C	0.7419523	-0.0356503	-0.0129492
C	2.8906532	0.2198314	-1.1210111
C	2.8584973	-0.5087509	1.0835861
C	1.4627635	-0.4461366	1.1312929
C	1.4937626	0.3007165	-1.1592558
H	3.5192177	0.4710111	-1.9905147
H	3.4500544	-0.8530118	1.9456920
H	0.9416718	-0.7491003	2.0508136
H	1.0013885	0.6510914	-2.0777791
C	-0.7419523	0.0356503	-0.0129492
N	-3.5594988	0.1792600	-0.0212937
C	-1.4937626	-0.3007165	-1.1592558
C	-1.4627635	0.4461366	1.1312929
C	-2.8584973	0.5087509	1.0835861
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H	-1.0013885	-0.6510914	-2.0777791
H	-0.9416718	0.7491003	2.0508136
H	-3.4500544	0.8530118	1.9456920
H	-3.5192177	-0.4710111	-1.9905147
Cl	-5.9884930	0.0088923	-2.1175979
Ga	-5.7976814	0.1969748	0.1004939
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C	-10.8344519	0.2230991	0.0414946
C	-8.6804786	1.3426414	-0.1124310
C	-8.7219809	-0.9056432	0.4678389
C	-10.1183342	-0.9419512	0.3942380
C	-10.0737807	1.3872264	-0.2121511
H	-8.0580790	2.2358228	-0.2773298
H	-8.1250359	-1.7902470	0.7407780
H	-10.6405880	-1.8900650	0.5871007
H	-10.5636788	2.3394769	-0.4610277
C	-12.3167464	0.2242536	-0.0598036
N	-15.1528589	0.2196439	-0.2620018
C	-12.9898002	1.0073145	-1.0236416
C	-13.1173842	-0.5604192	0.7995387
C	-14.5138243	-0.5226557	0.6582054
C	-14.3920315	0.9647273	-1.0817912
H	-12.4286957	1.6222869	-1.7433137
H	-12.6620937	-1.1745947	1.5910593
H	-15.1501348	-1.1252810	1.3309081
H	-14.9285795	1.5649486	-1.8383095

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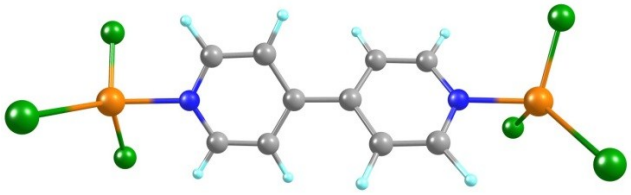

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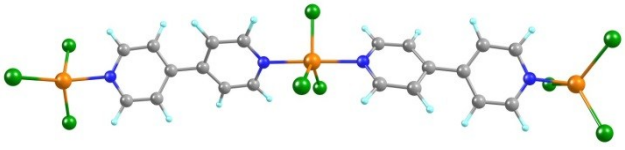
	X	Y	Z
C	0.0105756	0.7430315	0.0177486
C	0.3849160	1.4678790	-1.1361478
C	0.3935866	2.8643620	-1.1031445
N	0.0430035	3.5504748	0.0065149
C	-0.3094941	2.8814255	1.1260800
C	-0.3378892	1.4850934	1.1688876
H	0.7022141	0.9537137	-2.0543162
H	0.7056449	3.4758435	-1.9650933
H	-0.5575416	3.5048168	2.0000201
H	-0.6549761	0.9857893	2.0953098
C	-0.0105756	-0.7430315	0.0177486
C	0.3378892	-1.4850934	1.1688876
C	0.3094941	-2.8814255	1.1260800
N	-0.0430035	-3.5504748	0.0065149
C	-0.3935866	-2.8643620	-1.1031445
C	-0.3849160	-1.4678790	-1.1361478
H	0.6549761	-0.9857893	2.0953098
H	0.5575416	-3.5048168	2.0000201
H	-0.7056449	-3.4758435	-1.9650933
H	-0.7022141	-0.9537137	-2.0543162
Ga	-0.0259933	5.6409971	-0.0330379
Cl	-2.0852225	6.0531846	-0.6123830
Cl	0.4671546	6.0973533	2.0472158
Cl	1.4882146	6.0518379	-1.5576540
Ga	0.0259933	-5.6409971	-0.0330379
Cl	2.0852225	-6.0531846	-0.6123830
Cl	-0.4671546	-6.0973533	2.0472158
Cl	-1.4882146	-6.0518379	-1.5576540

$(GaCl_3)_3(bipy)_2\ (C_2)$



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N	9.1969276	-1.4023139	-0.2931462
C	7.2702155	-1.2057448	1.1253218
C	7.0176851	-1.1907202	-1.2758632
C	8.4026821	-1.3322937	-1.3843022
C	8.6466340	-1.3532151	0.9405125
H	6.8658863	-1.1903373	2.1472505
H	6.4151247	-1.1117584	-2.1916294
H	8.9179260	-1.4025383	-2.3557699
H	9.3488009	-1.4564265	1.7831545
Ga	11.2686952	-1.4723094	-0.5075356
N	2.1674888	-0.5689302	0.3953230
C	4.0447341	-1.5425101	-0.7524588
C	4.4015422	-0.1633863	1.1932993
C	3.0147646	-0.0003112	1.2770575
C	2.6704105	-1.3341898	-0.5939135

H	4.3977925	-2.1929723	-1.5655771
H	5.0469213	0.3473395	1.9223355
H	2.5474007	0.5985447	2.0745196
H	1.9255127	-1.7937453	-1.2632518
Ga	0.0000000	0.0000000	0.4187307
Cl	11.8348741	0.6321513	-0.4485802
Cl	11.4652175	-2.4325642	-2.4635906
Cl	11.8232320	-2.6403200	1.2561771
N	-2.1674888	0.5689302	0.3953230
Cl	0.5653067	1.8391584	-0.7059868
Cl	0.0000000	0.0000000	2.6504774
Cl	-0.5653067	-1.8391584	-0.7059868
C	-4.9494184	0.9431181	0.1505256
C	-3.0147646	0.0003112	1.2770575
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H	-1.9255127	1.7937453	-1.2632518
H	-4.3977925	2.1929723	-1.5655771
H	-5.0469213	-0.3473395	1.9223355
C	-6.4173612	1.1155960	0.0015243
N	-9.1969276	1.4023139	-0.2931462
C	-7.0176851	1.1907202	-1.2758632
C	-7.2702155	1.2057448	1.1253218
C	-8.6466340	1.3532151	0.9405125
C	-8.4026821	1.3322937	-1.3843022
H	-6.4151247	1.1117584	-2.1916294
H	-6.8658863	1.1903373	2.1472505
H	-9.3488009	1.4564265	1.7831545
H	-8.9179260	1.4025383	-2.3557699
Ga	-11.2686952	1.4723094	-0.5075356
Cl	-11.8348741	-0.6321513	-0.4485802
Cl	-11.4652175	2.4325642	-2.4635906
Cl	-11.8232320	2.6403200	1.2561771

$[Ga_4Cl_8bipy_{12}]^{4+}([GaCl_4]^-)_4$ (C_1)

	X	Y	Z
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Ga	-5.9501751	-2.3092184	-4.5865623
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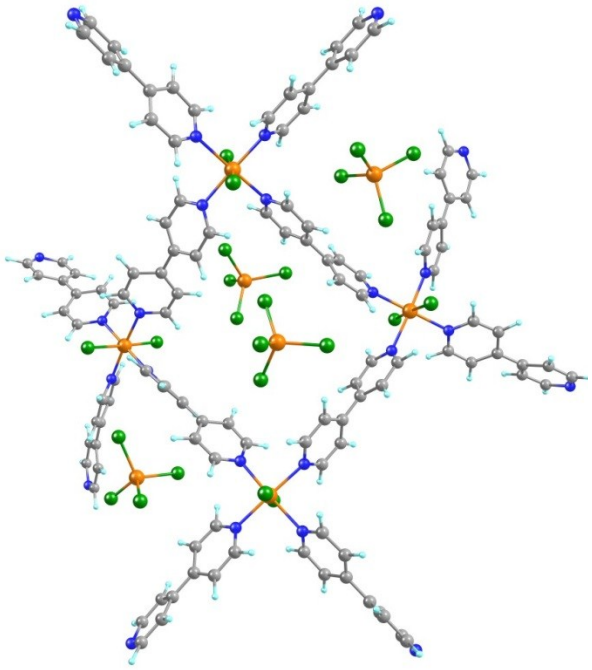
N	-8.0294584	-2.5276899	-4.0240164
N	-3.8378009	-1.9848214	-5.0956951
N	-6.3614266	-3.3840250	-6.5402076
N	-5.5993551	-1.3244013	-2.7312642
C	-4.9292904	-0.1690727	-0.2584453
C	-5.8124832	-2.0010693	-1.5769164
C	-5.0867508	-0.0707085	-2.6710246
C	-4.7421624	0.5401480	-1.4620693
C	-5.4839955	-1.4652179	-0.3345447



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H	-5.7131087	-2.0367542	0.5746832
C	-4.6302741	0.4058201	1.0737937
C	-1.2327754	-0.9822312	-5.4893736
C	-2.9100659	-2.0699786	-4.1151010
C	-3.4740950	-1.4625413	-6.2870215
C	-2.1837375	-0.9865161	-6.5327918
C	-1.6167140	-1.5587241	-4.2596573
H	-3.2270499	-2.5402610	-3.1722820
H	-4.2690041	-1.3787474	-7.0426282
H	-1.9542852	-0.5423876	-7.5119431
H	-0.9358465	-1.6040441	-3.3974114
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C	-4.0321321	0.0908397	3.3982862
H	-3.7655352	-1.4329140	1.9033561
H	-5.3073849	2.4413174	0.6293882
H	-5.0264331	3.2188902	3.0031291
H	-3.6958060	-0.5518623	4.2220732
Ga	-4.5441439	1.9544563	5.7422458
N	2.6036678	0.9178483	-5.9578971
C	0.6493553	0.4399905	-4.6256918
C	0.8344596	-0.4439224	-6.8631229
C	2.0857315	0.1730328	-6.9611734
C	1.8812407	1.0695019	-4.8227124
H	0.1190710	0.6214602	-3.6784794
H	0.4624349	-1.0363879	-7.7114732
H	2.7232962	0.0481578	-7.8488832
H	2.2937349	1.7326708	-4.0475652
Ga	4.6395019	1.6745811	-6.0116813
N	-4.6960179	2.5600445	7.8963367
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N	-2.4151120	1.2348065	5.9951849
Cl	-3.7685430	4.1067795	5.3040437
Cl	-5.3409295	-0.1224093	6.3898365
N	6.7120579	2.3716410	-5.9203615
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N	4.3418364	2.6228230	-8.0389246
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H	0.6758465	2.0390623	4.8551167
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C	-3.8053773	3.4032314	8.4613879
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H	-3.1184927	4.4688612	10.2082651
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C	-5.1159249	3.7803221	12.0189380
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H	-6.2914683	2.7465318	15.0751913
C	7.2989324	-2.5749859	9.5888557
C	6.0051025	-3.0988175	7.5923722
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H	8.2362246	-0.8131457	6.7790807
H	8.8788777	-1.1083631	9.1907675
H	5.6221881	-3.9856914	9.5225155
C	7.6088680	-2.7555119	11.0311005
N	8.2066519	-3.1028713	13.7888121
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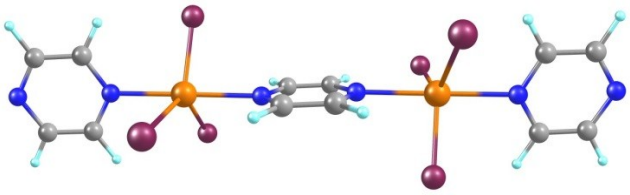
C	10.2145182	-3.7905596	4.4821550
H	8.2473234	-4.1176851	5.3728294
H	8.4157199	-0.8513289	2.7738381
H	10.7667632	-1.3240601	2.1773691
H	10.6726555	-4.6305571	5.0232727
C	12.4087135	-3.2680580	3.3232589
N	15.1729336	-3.7586270	2.8544378
C	13.2769933	-2.2478507	2.8743503
C	12.9789424	-4.5457052	3.5212578

C	14.3481877	-4.7324647	3.2747724
C	14.6319177	-2.5441470	2.6588795
H	12.9128061	-1.2238350	2.7080436
H	12.3644943	-5.4009682	3.8386905
H	14.8013810	-5.7291068	3.4230541
H	15.3169325	-1.7512927	2.3093833
C	4.0876142	3.9259335	-10.5477894
C	3.3760167	3.5472759	-8.2463385
C	5.1722528	2.3252009	-9.0637131
C	5.0855970	2.9527403	-10.3109485
C	3.2116357	4.2023269	-9.4726549
H	2.7358455	3.7772347	-7.3805618
H	5.9193243	1.5426003	-8.8588540
H	5.8179051	2.6943084	-11.0887678
H	2.3874862	4.9218150	-9.5833687
C	3.9779295	4.6256278	-11.8567494
N	3.8050512	5.9747205	-14.3576052
C	3.4978839	5.9516229	-11.9519935
C	4.3634232	4.0011033	-13.0647626
C	4.2564330	4.7121449	-14.2709940
C	3.4357326	6.5709507	-13.2114802
H	3.2008991	6.5148830	-11.0546172
H	4.7222055	2.9612845	-13.0771538
H	4.5513458	4.2308207	-15.2207491
H	3.0712328	7.6104626	-13.2951160
C	9.3595972	3.2927973	-5.4862627
C	7.6971369	1.5137789	-5.5628413
C	7.0270393	3.6788921	-6.0802204
C	8.3229371	4.1657458	-5.8945440
C	9.0104415	1.9317009	-5.3255960
H	7.4161908	0.4562443	-5.4520939
H	6.1879873	4.3505873	-6.3159639
H	8.5059575	5.2424456	-6.0191784
H	9.7463916	1.1822605	-5.0013455
C	10.7329358	3.7921042	-5.2087839
N	13.3378941	4.7798011	-4.6330923
C	11.2480166	4.9424195	-5.8502411
C	11.5736179	3.1502551	-4.2715347
C	12.8498818	3.6841833	-4.0257743
C	12.5405399	5.3858876	-5.5292333
H	10.6631639	5.4822353	-6.6102066
H	11.2449146	2.2624182	-3.7072578
H	13.5091062	3.1942822	-3.2875189
H	12.9529240	6.2826034	-6.0261962
Ga	-0.2652672	-2.9889894	1.3960896
Cl	-1.4892394	-2.0241981	-0.1956735
Cl	-0.0567321	-5.1524783	1.0712917
Cl	-1.2871504	-2.6183536	3.3773732
Cl	1.7500150	-2.0213933	1.5226305

Ga	9.3978871	-0.8726294	-1.4111038
Cl	8.0599773	-1.1807900	-3.1709749
Cl	9.5857404	-2.8118105	-0.3461838
Cl	8.5261378	0.5903245	0.0397745
Cl	11.3372367	-0.0937200	-2.1517288
Ga	-9.1420217	-0.7606360	1.0104916
Cl	-9.4794961	-2.7263103	0.0360981
Cl	-10.9765526	0.0093379	2.0160058
Cl	-8.4629309	0.7093387	-0.5171772
Cl	-7.5802618	-1.0364115	2.5857397
Ga	-1.4568369	3.3735014	-2.5339585
Cl	-2.4048937	1.9278689	-3.9756803
Cl	-2.9233777	3.7502336	-0.9010389
Cl	-0.9266247	5.2151734	-3.6144181
Cl	0.3666883	2.3893421	-1.6968700

$(GaBr_3)_2pyz_3$ (staggered, C_i)



E = -20087.44120797

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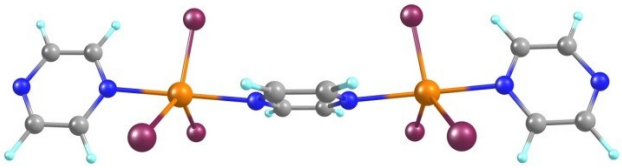
Br	-3.8165155	0.6866056	-2.0283809
Ga	-3.7224221	-0.1381396	0.2000136
Br	-3.8042454	1.3745331	2.0308303
Br	-3.4249534	-2.4650759	0.5757144
N	-5.9793057	-0.2689679	0.2807308
N	-1.3923644	0.0098421	0.0904192
N	1.3923644	-0.0098421	-0.0904192
C	-0.7685124	-0.5491091	-0.9625180
C	-0.6311250	0.5589003	1.0544752
C	0.7685124	0.5491091	0.9625180
C	0.6311250	-0.5589003	-1.0544752
H	-1.4008752	-0.9877525	-1.7496098
H	-1.1617650	1.0152451	1.9056570
H	1.4008752	0.9877525	1.7496098
H	1.1617650	-1.0152451	-1.9056570
N	-8.7779636	-0.2497370	0.5079860
C	-6.6383849	-1.3058635	0.8310843
C	-6.7060438	0.7789289	-0.1565093
C	-8.1049281	0.7766359	-0.0374353
C	-8.0402970	-1.2841510	0.9382634
H	-6.0252090	-2.1549699	1.1743255
H	-6.1545538	1.6145526	-0.6150189
H	-8.6929493	1.6373977	-0.3990803
H	-8.5736558	-2.1390328	1.3881516
Br	3.8042454	-1.3745331	-2.0308303
Ga	3.7224221	0.1381396	-0.2000136
Br	3.4249534	2.4650759	-0.5757144
Br	3.8165155	-0.6866056	2.0283809
N	5.9793057	0.2689679	-0.2807308
N	8.7779636	0.2497370	-0.5079860
C	6.7060438	-0.7789289	0.1565093
C	6.6383849	1.3058635	-0.8310843

C	8.0402970	1.2841510	-0.9382634
C	8.1049281	-0.7766359	0.0374353
H	6.1545538	-1.6145526	0.6150189
H	6.0252090	2.1549699	-1.1743255
H	8.5736558	2.1390328	-1.3881516
H	8.6929493	-1.6373977	0.3990803

$(GaBr_3)_2pyz_3$ (eclipsed, C_s)



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Br	-2.2444689	-0.3837102	3.3581873
Ga	0.0702065	-0.0010183	3.7240447
Br	0.9296479	2.2085423	3.9013967
Br	1.5746660	-1.8403980	3.7999772
N	-0.1248635	-0.0537139	5.9769675
N	0.2740739	0.0585403	1.3957191
N	0.2740739	0.0585403	-1.3957191
C	0.2888376	-1.0949325	0.7006105
C	0.2570561	1.2100945	0.7019031
C	0.2570561	1.2100945	-0.7019031
C	0.2888376	-1.0949325	-0.7006105
H	0.3180742	-2.0302834	1.2811794
H	0.2573743	2.1439824	1.2868760
H	0.2573743	2.1439824	-1.2868760
H	0.3180742	-2.0302834	-1.2811794
N	-0.2234509	0.0023150	8.7819691
C	1.0044939	-0.0138604	6.7125987
C	-1.3015539	-0.0657468	6.6300573
C	-1.3370876	-0.0375670	8.0358182
C	0.9422636	0.0137631	8.1145163
H	1.9605459	-0.0110935	6.1662212
H	-2.2107681	-0.1023917	6.0078232
H	-2.3055056	-0.0482950	8.5648414
H	1.8704587	0.0457732	8.7100504
Br	1.5746660	-1.8403980	-3.7999772
Ga	0.0702065	-0.0010183	-3.7240447
Br	-2.2444689	-0.3837102	-3.3581873
Br	0.9296479	2.2085423	-3.9013967
N	-0.1248635	-0.0537139	-5.9769675
N	-0.2234509	0.0023150	-8.7819691
C	1.0044939	-0.0138604	-6.7125987
C	-1.3015539	-0.0657468	-6.6300573
C	-1.3370876	-0.0375670	-8.0358182
C	0.9422636	0.0137631	-8.1145163
H	1.9605459	-0.0110935	-6.1662212
H	-2.2107681	-0.1023917	-6.0078232
H	-2.3055056	-0.0482950	-8.5648414
H	1.8704587	0.0457732	-8.7100504

$[Ga_4Br_8pyz_{12}]^{4+}([GaBr_4]^-)_4$ (C_1)

	X	Y	Z
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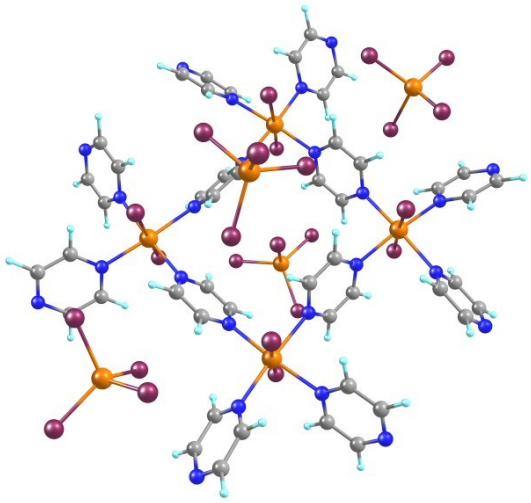

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Ga	-5.1322907	0.1029305	-0.0239332
N	-3.3354267	-1.3408428	-0.2202952
N	-3.7424836	1.8233724	-0.0917333
N	-6.4623398	-1.7891758	0.0213857
Br	-5.3590792	0.0914222	-2.4829592
N	-1.7584250	3.7972231	-0.1222565
C	-3.5825785	2.6660723	0.9515413
C	-2.9533149	2.0048225	-1.1698389
C	-1.9600435	2.9907072	-1.1851215
C	-2.5880808	3.6594477	0.9349615
H	-4.2440671	2.5483392	1.8231986
H	-3.1018535	1.3563604	-2.0459891
H	-1.3244943	3.1206754	-2.0730663
H	-2.4578096	4.3372870	1.7923634
Ga	-0.0442227	5.1811449	-0.1088948
N	-1.3579364	-3.3257412	-0.3003165
C	-2.3726193	-1.4019091	0.7189855
C	-3.2669258	-2.2240903	-1.2408862
C	-2.2778368	-3.2123172	-1.2838809
C	-1.3794675	-2.4030099	0.6802788
H	-2.3977832	-0.6725366	1.5454251
H	-4.0180815	-2.1243740	-2.0394306
H	-2.2088257	-3.9246402	-2.1203099
H	-0.6201364	-2.4647638	1.4776779
Ga	0.0715397	-5.1422729	-0.2273281
N	1.8393253	6.5396730	-0.1250296
N	-1.2554938	6.9780884	-0.0045159
N	1.3976010	3.3710028	-0.2519012
Br	-0.0338689	5.3361578	-2.5697019
Br	0.1557514	5.0723418	2.3212871
N	1.2960809	-6.9512935	-0.1970572
N	1.7780227	-3.7343322	-0.2938765
N	-1.8161625	-6.4670036	-0.1782130
Br	0.0086486	-5.2732796	-2.6824266
Br	0.0148198	-5.0686386	2.1968772
N	3.7514935	-1.7577131	-0.2617662
C	2.6932107	-3.6842740	0.6946763
C	1.8731922	-2.8288968	-1.2921570
C	2.8610162	-1.8376877	-1.2755140
C	3.6876621	-2.6895936	0.7105779
H	2.6365066	-4.4342241	1.4998296
H	1.1483582	-2.8893071	-2.1192097
H	2.9323967	-1.0980640	-2.0876773
H	4.4288710	-2.6527381	1.5253737
Ga	5.1673151	-0.0756244	-0.1683362
N	3.3652868	1.3746634	-0.2783230
C	1.4467231	2.4265898	0.7102015
C	2.2725650	3.2630035	-1.2715460
C	3.2570512	2.2642338	-1.2858832

C	2.4337835	1.4243848	0.6967671
H	0.7117206	2.4686597	1.5323084
H	2.1774542	3.9882909	-2.0944233
H	3.9699288	2.1708763	-2.1193801
H	2.4729298	0.6752938	1.5067287
N	6.5284234	1.7969422	-0.1101712
N	6.9531801	-1.3171813	-0.0723570
Br	5.3510041	-0.0251047	-2.6196690
Br	5.0368696	0.0199749	2.2647398
N	8.2176011	4.0439073	-0.0156505
C	6.4094626	2.7206572	0.8656879
C	7.4900288	1.9885766	-1.0365310
C	8.3346348	3.1111061	-0.9731754
C	7.2535586	3.8441019	0.8961608
H	5.6489128	2.5273796	1.6392000
H	7.5590291	1.2416661	-1.8433434
H	9.1263131	3.2512398	-1.7286933
H	7.1441319	4.5971102	1.6951925
N	9.3581967	-2.7659339	-0.0775538
C	7.9092664	-1.0881372	0.8553787
C	7.1672649	-2.3080640	-0.9619121
C	8.3701392	-3.0377367	-0.9399282
C	9.1143074	-1.8051710	0.8269928
H	7.6911560	-0.3284115	1.6207923
H	6.3860711	-2.5016684	-1.7096517
H	8.5227706	-3.8599124	-1.6580673
H	9.9040103	-1.5849819	1.5648873
N	2.7047894	-9.3781810	-0.2837349
C	1.0572578	-7.9302007	0.7031717
C	2.2787146	-7.1540491	-1.0979962
C	2.9893901	-8.3680072	-1.1160646
C	1.7529140	-9.1464027	0.6330844
H	0.3069096	-7.7211456	1.4805058
H	2.4786234	-6.3541904	-1.8240021
H	3.8060023	-8.5118794	-1.8424152
H	1.5224891	-9.9549705	1.3470465
N	-4.0765100	-8.1354933	-0.0696232
C	-2.7285717	-6.3428877	0.8079517
C	-2.0268526	-7.4197347	-1.1094723
C	-3.1560473	-8.2545468	-1.0389270
C	-3.8589708	-7.1777433	0.8449665
H	-2.5227225	-5.5870308	1.5831631
H	-1.2887972	-7.4898842	-1.9243587
H	-3.3112093	-9.0410196	-1.7970271
H	-4.6023031	-7.0659881	1.6525260
N	-8.1196342	-4.0588506	0.1194976
C	-6.2948440	-2.7355852	0.9683052
C	-7.4540685	-1.9700440	-0.8747202
C	-8.2823466	-3.1044066	-0.8097473

C	-7.1246810	-3.8698500	1.0001569
H	-5.5068396	-2.5555444	1.7174569
H	-7.5616933	-1.2041555	-1.6591940
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H	-6.9770898	-4.6410087	1.7752825
N	-2.6786253	9.3981355	-0.0031780
C	-2.2689748	7.1901553	-0.8689693
C	-0.9930653	7.9426396	0.9054747
C	-1.6979188	9.1549161	0.8799057
C	-2.9848721	8.4013002	-0.8435005
H	-2.4927594	6.4011161	-1.5996396
H	-0.2155286	7.7259973	1.6532382
H	-1.4504036	9.9512804	1.6017722
H	-3.8247144	8.5527949	-1.5411058
N	4.0895206	8.2271104	-0.1174167
C	2.8073329	6.4101776	0.8048925
C	1.9889629	7.5104701	-1.0494080
C	3.1134460	8.3543381	-1.0293108
C	3.9318283	7.2532514	0.7920231
H	2.6494217	5.6423202	1.5789944
H	1.2068763	7.5880458	-1.8210946
H	3.2184853	9.1543784	-1.7817773
H	4.7215937	7.1348148	1.5534535
Br	-4.9674590	-0.0388434	2.3934783
N	-9.3480557	2.7558985	0.1759706
C	-7.1697701	2.3296283	-0.7548249
C	-7.8755667	1.0638245	1.0450475
C	-9.0844735	1.7752541	1.0533996
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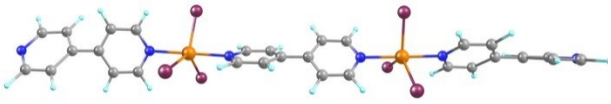
H	-6.4009643	2.5472599	-1.5086750
H	-7.6400687	0.2884430	1.7895496
H	-9.8606743	1.5339387	1.7990142
H	-8.5440995	3.8902300	-1.3924124
Ga	-0.4676749	-0.6175104	4.4077555
Br	-2.1584783	-2.2862312	4.2205860
Br	0.1177823	-0.1633549	6.6177874
Br	-1.2320537	1.3679129	3.2806039
Br	1.4329943	-1.3472215	3.1185341
Ga	-0.0642632	0.2052807	-4.0448037
Br	-0.4914425	-2.0043892	-4.7388327
Br	-0.0720120	0.1336128	-1.5954933
Br	-1.7514181	1.7079195	-4.7241864
Br	2.0987765	0.9486545	-4.6376696
Ga	6.0135948	-6.0561365	1.2113814
Br	7.7027034	-7.6540414	0.9878074
Br	4.0654051	-6.8687326	2.3074417
Br	5.3418820	-5.3428185	-1.0173892
Br	6.7059060	-4.1085562	2.4005492
Ga	-5.9142904	6.0239263	1.4140428

Br	-7.5637176	7.6650804	1.1955742
Br	-6.6465596	4.0887214	2.5894599
Br	-3.9549848	6.7967355	2.5278013
Br	-5.2582205	5.3239052	-0.8233051

$(GaBr_3)_2bipy_3$ (eclipsed, C_2)



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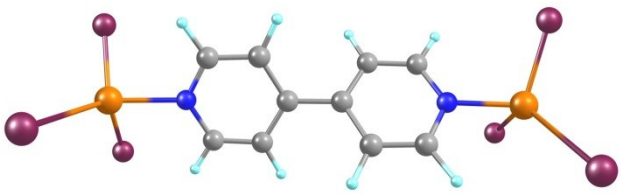
Br	5.7209200	-2.3591572	0.7686538
Br	5.6251513	1.6796597	1.5583409
N	8.0862925	-0.1433159	0.1498306
N	3.5655053	-0.0917834	-0.1833613
C	10.9130366	-0.2094664	0.1052964
C	8.8067025	0.8798798	0.6514077
C	8.7438395	-1.1990238	-0.3760318
C	10.1384869	-1.2700550	-0.4176481
C	10.2060684	0.8843095	0.6504985
H	8.2225079	1.7165047	1.0674834
H	8.1163464	-2.0187709	-0.7588719
H	10.6165438	-2.1676528	-0.8349935
H	10.7378839	1.7577192	1.0541623
C	12.3981652	-0.2447070	0.0822854
N	15.2407062	-0.3115680	0.0375940
C	13.1674472	0.3407374	1.1121422
C	13.1062939	-0.8649434	-0.9708162
C	14.5101832	-0.8661667	-0.9444994
C	14.5682388	0.2760927	1.0416640
H	12.6833906	0.8184886	1.9771284
H	12.5735136	-1.3189732	-1.8198688
H	15.0740180	-1.3403938	-1.7678154
H	15.1793548	0.7222341	1.8467006
C	0.7423960	-0.0194820	-0.1876234
C	2.8897669	0.2777550	-1.2885236
C	2.8660713	-0.4266637	0.9215949
C	1.4695616	-0.4015881	0.9626402
C	1.4907463	0.3235873	-1.3336839
H	3.5102967	0.5436763	-2.1599442
H	3.4582091	-0.7349288	1.7968487
H	0.9541230	-0.7078546	1.8841033
H	0.9952455	0.6551121	-2.2574961
C	-0.7423960	0.0194820	-0.1876234
N	-3.5655053	0.0917834	-0.1833613
C	-1.4907463	-0.3235873	-1.3336839
C	-1.4695616	0.4015881	0.9626402
C	-2.8660713	0.4266637	0.9215949
C	-2.8897669	-0.2777550	-1.2885236
H	-0.9952455	-0.6551121	-2.2574961
H	-0.9541230	0.7078546	1.8841033
H	-3.4582091	0.7349288	1.7968487

H	-3.5102967	-0.5436763	-2.1599442
Br	-6.1180619	-0.3311629	-2.3500134
Ga	-5.8377740	0.1050546	-0.0171840
Br	-5.6251513	-1.6796597	1.5583409
Br	-5.7209200	2.3591572	0.7686538
N	-8.0862925	0.1433159	0.1498306
C	-10.9130366	0.2094664	0.1052964
C	-8.7438395	1.1990238	-0.3760318
C	-8.8067025	-0.8798798	0.6514077
C	-10.2060684	-0.8843095	0.6504985
C	-10.1384869	1.2700550	-0.4176481
H	-8.1163464	2.0187709	-0.7588719
H	-8.2225079	-1.7165047	1.0674834
H	-10.7378839	-1.7577192	1.0541623
H	-10.6165438	2.1676528	-0.8349935
C	-12.3981652	0.2447070	0.0822854
N	-15.2407062	0.3115680	0.0375940
C	-13.1062939	0.8649434	-0.9708162
C	-13.1674472	-0.3407374	1.1121422
C	-14.5682388	-0.2760927	1.0416640
C	-14.5101832	0.8661667	-0.9444994
H	-12.5735136	1.3189732	-1.8198688
H	-12.6833906	-0.8184886	1.9771284
H	-15.1793548	-0.7222341	1.8467006
H	-15.0740180	1.3403938	-1.7678154

$(GaBr_3)_2$bipy (C_2)



E = -19790.04723484

	X	Y	Z
C	0.1352531	0.7304990	-0.0131617
C	-0.1352531	-0.7304990	-0.0131617
N	-0.6505212	-3.4922928	-0.0154835
C	-0.6375518	-1.3822158	-1.1615500
C	0.1037032	-1.5221061	1.1326380
C	-0.1608697	-2.8934863	1.0926587
C	-0.8843369	-2.7567539	-1.1245110
H	-0.8641880	-0.8234832	-2.0805403
H	0.5243293	-1.0856026	2.0496878
H	0.0333097	-3.5548133	1.9527844
H	-1.2703552	-3.3089661	-1.9968069
Ga	-1.1767206	-5.5313955	0.0289787
N	0.6505212	3.4922928	-0.0154835
C	-0.1037032	1.5221061	1.1326380
C	0.6375518	1.3822158	-1.1615500
C	0.8843369	2.7567539	-1.1245110
C	0.1608697	2.8934863	1.0926587
H	-0.5243293	1.0856026	2.0496878
H	0.8641880	0.8234832	-2.0805403
H	1.2703552	3.3089661	-1.9968069
H	-0.0333097	3.5548133	1.9527844
Ga	1.1767206	5.5313955	0.0289787

Br	3.3727297	5.4100672	0.8036780
Br	-0.3787593	6.3896220	1.5446071
Br	0.9194853	6.1393328	-2.2129793
Br	-0.9194853	-6.1393328	-2.2129793
Br	-3.3727297	-5.4100672	0.8036780
Br	0.3787593	-6.3896220	1.5446071