**Molecular complexes of non-chelating polydentate Lewis bases
with group 13 Lewis acids: crystal structure and computed energy
of stepwise donor–acceptor bond formation**

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Synthetic procedures

All synthetic works were carried out using Schlenk line or InertLab 2GB glove box under argon. Dichloromethane (Vecton), deuterodichloromethane (Carl Roth, 99.6%D) and deuterochloroform (Carl Roth, 99.8%D) were dried over CaH_2. Toluene (Vecton) was dried over a mixture Na/K. All solvents were distilled, degassed by repetition of freezing-melting cycles under dynamic vacuum, stored over activated 4 Å zeolites prior to use. Trispentafluorophenylborane (ABCR, 97%), GaI_3 (obtained by direct reaction between the elements) and pyrazine (Sigma Aldrich, 99%) were purified by sublimation in vacuum. $E(C_6F_5)_3 \cdot Et_2O$ (E=Al, Ga, In) were synthesized according to Pohlmann and Brinckmann[S1]. **Caution!** Heating of complexes $E(C_6F_5)_3$ (E = Al, Ga, In) with Et_2O and pyrazine should be made with care, due to the risk of explosion.

Synthesis of B(C_6F_5)$_3$·pyz*Tol (1). To a suspension of $B(C_6F_5)_3$ (94.4(2) mg, 0.183(1) mmol) in 3 ml of toluene a 2 ml of pyrazine (14.6(2) mg, 0.183(1) mmol) solution in toluene was added under stirring. After 2 minutes a clear solution was formed. Volatiles were removed under vacuum (2 hours, 10^{-1} – 10^{-2} torr) at room temperature. Colorless crystals of **1** were observed. Yield: 95.4(2) mg, 0.139(1) mmol, 76%. Attempts to remove solvent molecule by heating in vacuum (330-340K, 2 hour, 10^{-1} – 10^{-2} torr) result in formation of viscous liquid. ^{1}H NMR (CDCl$_3$): 2.39 (s, CH_3, toluene), 7.15-7.31 (m, C_6H_5, toluene), 8.60 (s, 2H, $B(C_6F_5)_3$·Pyz), 9.18 (d, $^3J_{HH}$ = 4.0 Hz, 2H, $B(C_6F_5)_3$·Pyz). ^{19}F{H} NMR (CDCl$_3$): -161.99 (td, $^3J_{FF}$ = 25.3 Hz, $^4J_{FF}$ = 8.7 Hz, m-F, $B(C_6F_5)_3$·Pyz), -154.81 (t, $^3J_{FF}$ = 20.9 Hz, p-F, $B(C_6F_5)_3$·Pyz), -131.06 (d, $^3J_{FF}$ = 26.1 Hz, o-F, $B(C_6F_5)_3$·Pyz). IR (KBr), cm^{-1}: w 317, m 348, w 375, m 467, w 504, m 572, w 614, m 633, m 677, w 705, m 743, m 763, m 796, w 823, m 866, s 985, w 1029, s 1089, s 1107, m 1168, m 1230, m 1288, m 1382, m 1423, s 1469, s 1521, m 1602, m 1648, w 1716, w 1720, w 2858, w 2924, w 3078, w 3114, w 3442.

Synthesis of {B(C_6F_5)$_3$}$_2$·pyz*2CH$_2$Cl$_2$ (2). To a solution of $B(C_6F_5)_3$ (102.4(2) mg, 0.2000(4) mmol) in 3 ml of dichloromethane a 1 ml of pyrazine (8.0(2) mg, 0.10(1) mmol) solution in dichloromethane was added under stirring. After 2 minutes a clear pale yellow solution was formed. Volatiles were removed under vacuum (1 hour, 10^{-1} – 10^{-2} torr) at room temperature. Yellow crystals of **2** were observed. Yield: 98.3(2) mg, 0.0827(2) mmol, 83%. Attempts to remove solvent molecule by heating in vacuum (330-340K, 2 hour, 10^{-1} – 10^{-2} torr) result in formation of viscous liquid. ^{1}H NMR (CDCl$_3$): 5.32 (s, CH_2Cl_2), 9.08 (s, $[B(C_6F_5)_3]_2$Pyz). ^{19}F{H} NMR (CDCl$_3$): -160.76 (br s, m-F, $[B(C_6F_5)_3]_2$Pyz), -152.43 (br s, p-F, $[B(C_6F_5)_3]_2$Pyz), -131.10 (br s, o-F, $[B(C_6F_5)_3]_2$Pyz). IR (KBr), cm^{-1}: w 317, w 348, w 576, w 608, w 638, m 662, m 690, m 745, m 765, m 791, m 862, s 983, s 1104, m 1266, s 1291, w 1317, m 1381, s 1470, s 1523, w 1605, s 1649, w 2923, w 3136, w 3464.

Synthesis of Al(C_6F_5)$_3$·pyz (3). Solution of $Al(C_6F_5)_3 \cdot Et_2O$ (120.6(2) mg, 200.2(2) mmol) in 3 ml of dichloromethane added dropwise to 1 ml of pyrazine (16.1(2) mg, 201.2(1) mmol) solution in dichloromethane under stirring. A clear solution was formed. Volatiles were removed under vacuum (2 hours, 10^{-1} – 10^{-2} torr) at room temperature. Colorless crystals of **3** were observed. Yield: 110.7(2) mg, 182.0(2) mmol, 91%. IR (KBr), cm^{-1}: w 326, w 420, w 443, w 504, w 530, w 563, w 583, w 613, w 674, w 718, m 796, m 840, s 955, m 1025, s 1072, m 1137, m 1181, m 1276, w 1357, m 11416, s 1454, s 1512, s 1534, m 1648, w 2857, w 2927.

Synthesis of {Al(C$_6$F$_5$)$_3$}$_2$·pyz. To a solution of Ga(C$_6$F$_5$)$_3$·Et$_2$O (98.9(2) mg, 0.153(3) mmol) in 3 ml of dichloromethane a 2 ml of pyrazine (6.1(2) mg, 0.076(2) mmol) solution in toluene was added under stirring. After 2 minutes a clear solution was formed. Volatiles were removed under vacuum (1 hour, $10^{-1} – 10^{-2}$ torr) at room temperature. Yield: 90.2(2) mg, 0.0738(2) mmol, 97%. IR (KBr), cm^{-1}: w 328, w 357, w 382, w 403, m 422, m 458, m 505, w 538, w 587, m 612, m 662, w 720, w 743, m 791, w 839, s 957, w 1019, s 1071, m 1137, m 1178, w 1232, s 1270, m 1358, m 1380, s 1459, s 1513, s 1534, m 1644, w 1703, w 2925, w 3448.

Synthesis of Ga(C$_6$F$_5$)$_3$·pyz (4). To a suspension of Ga(C$_6$F$_5$)$_3$·Et$_2$O (180.1(2) mg, 279.2(3) mmol) in 2 ml of toluene a 1 ml of pyrazine (26.2(2) mg, 327.5(3) mmol) solution in toluene was added under stirring. After 2 minutes a clear solution was formed. Volatiles were removed under vacuum (2 hours, $10^{-1} – 10^{-2}$ torr) at room temperature. Colorless crystals of **4** were observed. Yield: 170.6(2) mg, 262.1(2) mmol, 94%. IR (KBr), cm^{-1}: w 327, w 356, w 372, w 399, w 421, w 458, w 490, w 534, w 581, m 612, w 720, m 800, s 962, w 1025, s 1074, w 1128, w 1153, m 1232, m 1272, s 1365, m 1421, s 1466, s 1514, w 1544, w 1558, w 1575, m 1642, w 1670, m 1711, w 1736, w 2854, w 2923.

Synthesis of {Ga(C$_6$F$_5$)$_3$}$_2$·pyz (5). To a solution of Ga(C$_6$F$_5$)$_3$·Et$_2$O (98.9(2) mg, 0.153(3) mmol) in 3 ml of dichloromethane a 2 ml of pyrazine (6.1(2) mg, 0.076(2) mmol) solution in toluene was added under stirring. After 2 minutes a white precipitate was formed. Precipitate was filtered and washed with dichloromethane. Volatiles were removed under vacuum (2 hours, $10^{-1} – 10^{-2}$ torr) at room temperature. Yield: 90.2(2) mg, 0.0738(2) mmol, 97%. [Ga(C$_6$F$_5$)$_3$]$_2$Pyz is insoluble in benzene, chloroform, toluene and dichloromethane. Single crystals of **5** were obtained by sublimation in vacuum at 440-460 K. IR (KBr), cm^{-1}: w 319, m 370, m 482, m 612, w 722, w 744, m 806, s 961, m 1016, s 1073, m 1127, w 1157, s 1274, s 1367, s 1468, s 1516, w 1580, w 1615, s 1643, w 3157.

Synthesis of In(C$_6$F$_5$)$_3$·pyz complex. Method 1. Solution of In(C$_6$F$_5$)$_3$·Et$_2$O (132.4(2) mg, 0.2003(3) mmol) in 3 ml of dichloromethane added dropwise to 1 ml of pyrazine (16.1(2) mg, 0.2012(24) mmol) solution in dichloromethane under stirring. Addition of first drops of In(C$_6$F$_5$)$_3$·Et$_2$O solution result in white precipitate formation. Precipitate was filtered and washed with dichloromethane. Volatiles were removed under vacuum (2 hours, $10^{-1} – 10^{-2}$ torr) at room temperature. Yield: 104.1(2) mg. Compound is insoluble in benzene, chloroform, toluene and dichloromethane. IR (KBr), cm^{-1}: m 358, w 399, w 420, m 454, w 487, w 582, m 605, w 719, m 741, m 782, m 800, w 903, s 959, m 1009, s 1052, s 1075, m 1128, m 1153, w 1236, s 1268, w 1323, s 1361, m 1423, s 1464, s 1510, w 1609, s 1638, w 1711, w 2316, w 2348, w 2381, w 2855, w 2923, w 3060, w 3134.

Method 2. Solution of pyrazine (8.0(2) mg, 0.10(1) mmol) in 1 ml of dichloromethane added dropwise to 3 ml of In(C$_6$F$_5$)$_3$·Et$_2$O (132.6(2) mg, 0.2006(3) mmol) solution in dichloromethane under stirring. Addition of first drops of pyrazine solution result in white precipitate formation. Precipitate was filtered and washed with dichloromethane. Volatiles were removed under vacuum (2 hours, $10^{-1} – 10^{-2}$ torr) at room temperature. Yield: 115.4(2) mg. Sample insoluble in benzene, chloroform, toluene and dichloromethane. IR (KBr), cm^{-1}: w 305, m 358, m 457, w 487, m 605, w 718, m 741, m 783, m 804, m 830, w 907, s 958, m 1010, s 1054, s 1076, m 1129, m 1154, m 1176, s 1267, w 1325, s 1360, s 1464, s 1511, m 1534, w 1609, s 1639, w 1690, w 1709, w 2322, w 2576, w 2856, w 2922, w 3065, w 3136.

Synthesis of {In(C₆F₅)₃}₂·pyz (6). Single crystals of **6** were obtained by sublimation of the precipitate of $In(C_6F_5)_3 \cdot pyz$ in vacuum at 440-460 K. For **6** IR (KBr), cm⁻¹: m 313, w 400, w 449, w 605, w 646, w 783, w 804, m 849, s 959, m 1009, s 1053, s 1074, m 1132, w 1186, m 1267, m 1361, s 1463, s 1510, m 1638, m 2361, m 2433, w 2854, w 2923, w 2952, w 3007, w 3450.

Formation of **6** can be explained by pyrazine elimination during sublimation of $In(C_6F_5)_3 \cdot pyz$ precipitate. IR spectra of $In(C_6F_5)_3 \cdot pyz$ precipitate obtained by methods 1 (Figure 11S) and 2 (Figure 12S) are similar to each other but are different from IR spectra of **6** (Figure 13S). The XRD pattern of precipitate differs from calculated for **6** from the crystal structure data (Figure 21S). Mass-spectrometric data of $In(C_6F_5)_3 \cdot pyz$ precipitate indicate pyrazine loss at 370-380 K without significant In-containing ions observed.

Synthesis of (GaI₃)₂·pyz (7). To avoid hydrolysis, all manipulations were carried out in wholeglass systems under vacuum. The molecular complex $(GaI_3)_2pyz$ was obtained by direct reaction between the components in slight excess of GaI_3. Pyz (14.7 mg, 0.18 mmol) was sublimed at 50 °C to GaI_3 (201.2 mg, 0.45 mmol) in the vacuumed reaction vessel. Reaction started immediately upon the condensation of pyrazine on the GaI_3. In order to complete the reaction, the system was heated to 120-150 °C for several hours. Yellow diaphanous single crystals, suitable for X-ray analysis, were grown at 100-110 °C for several days.

NMR spectra

NMR spectroscopy studies were performed on a Bruker AVANCE 400 instrument at room temperature. TMS and $CFCl_3$ were used as external standards. The resonance frequency in ^1H NMR is 400 MHz, in $^{19}F\{H\}$ NMR is 376.5 MHz. Chemical shifts are given in ppm.
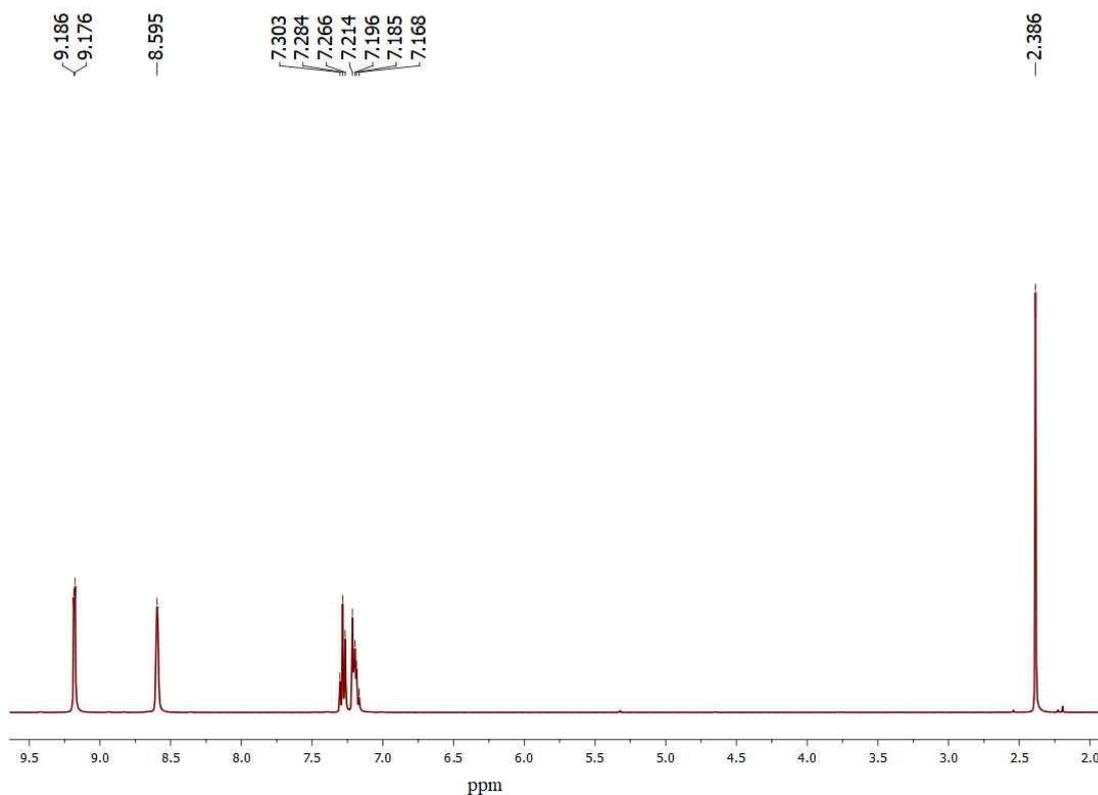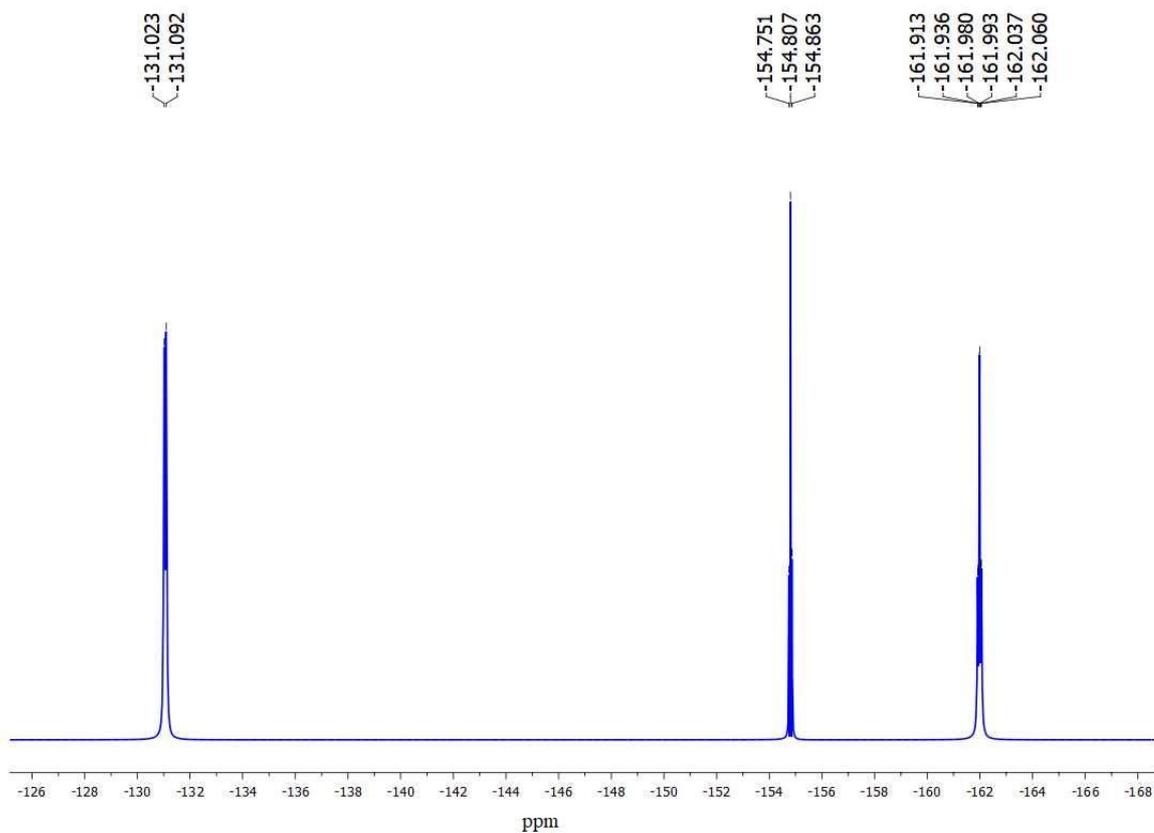

Figure S1 ^1H NMR of **1** in $CDCl_3$.

Figure S2 $^{19}F\{^1H\}$ NMR of **1** in $CDCl_3$.
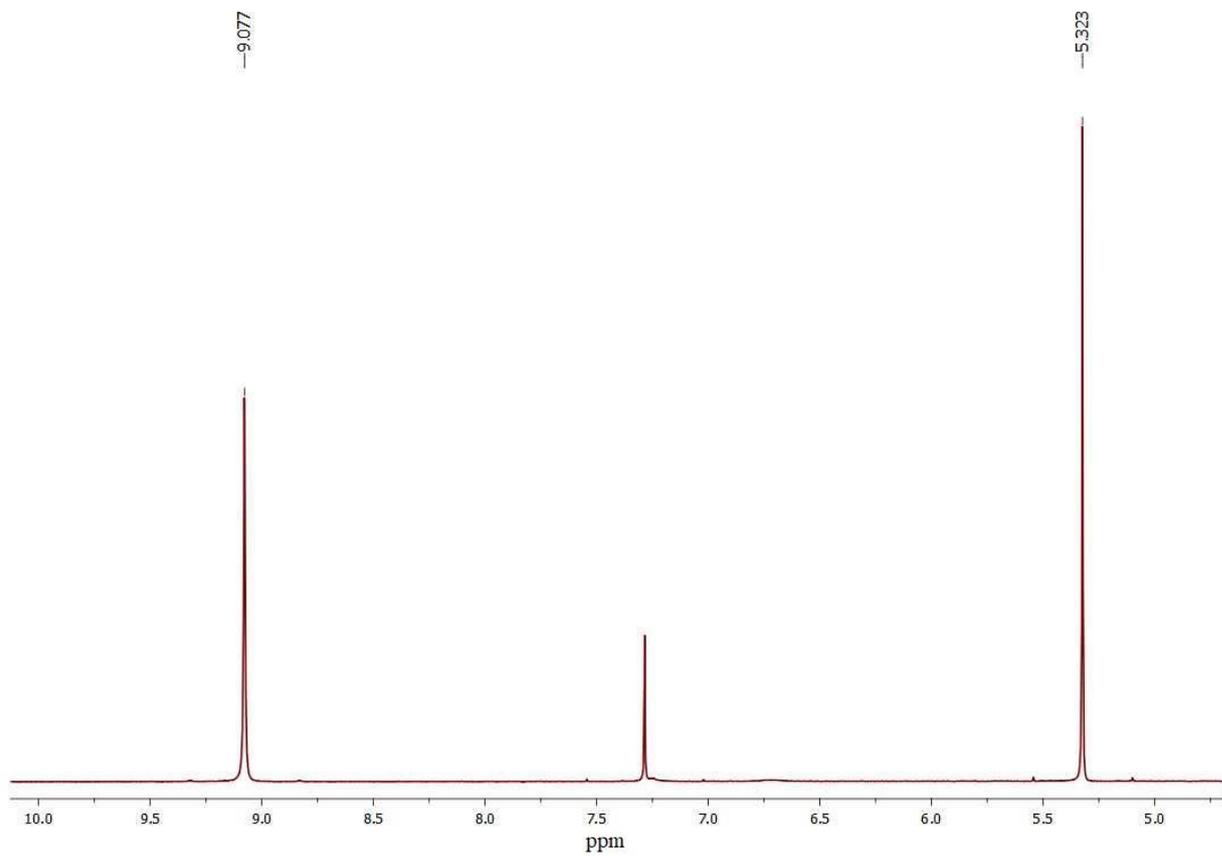
Figure S3 ^{1}H NMR of **2** in CDCl$_3$.

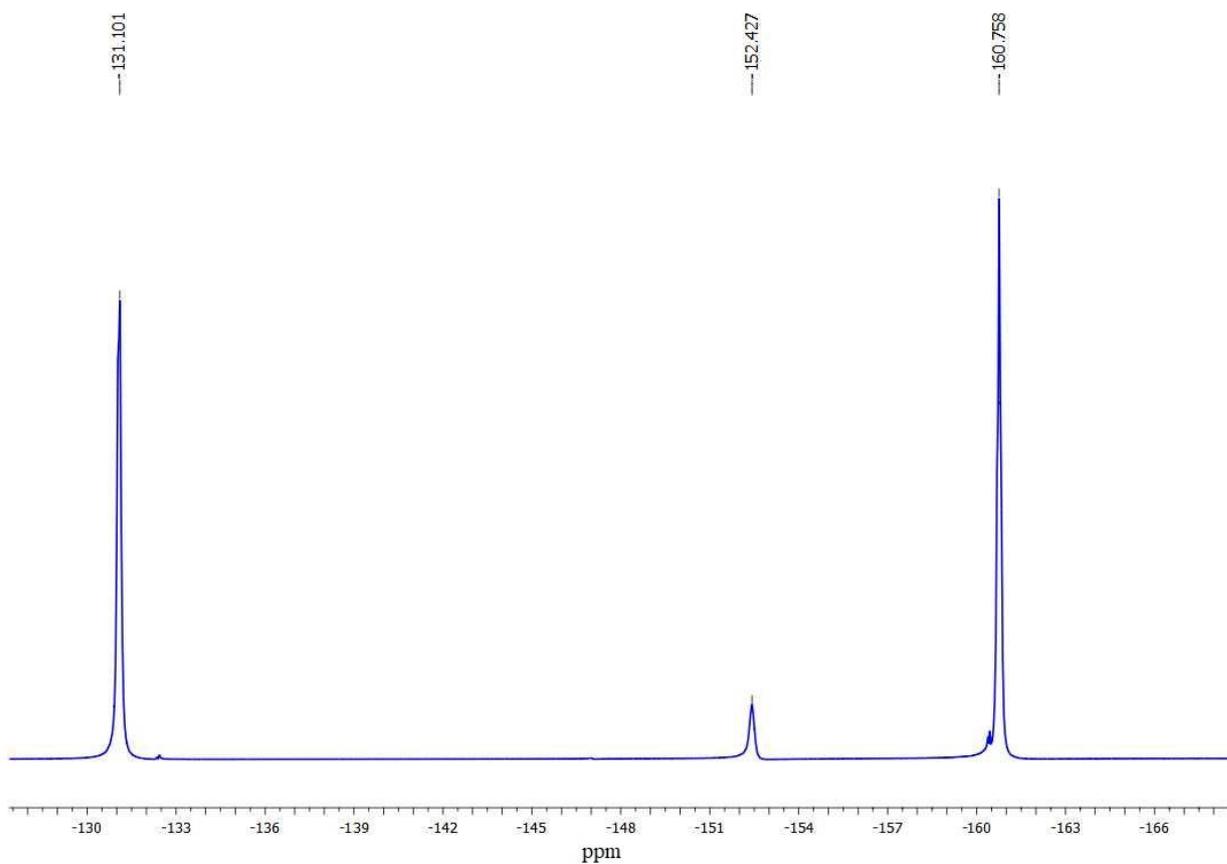**Figure S4** ^{19}F{^{1}H} NMR of **2** in CDCl$_3$.

IR spectra

IR spectra in the range 300-4000 cm^{-1} were recorded on a Shimadzu IR Prestige–21 FTIR spectrometer in KBr discs. Samples were prepared for IR spectroscopic studies in the glove box INERTLAB 2GB under argon atmosphere. The IR spectra for the each sample were recorded immediately after sample preparation. Adaptive baseline correction was performed using SpectraGryph v1.2.15 software developed by Dr. Friedrich Menges (http://spectragryph.com).
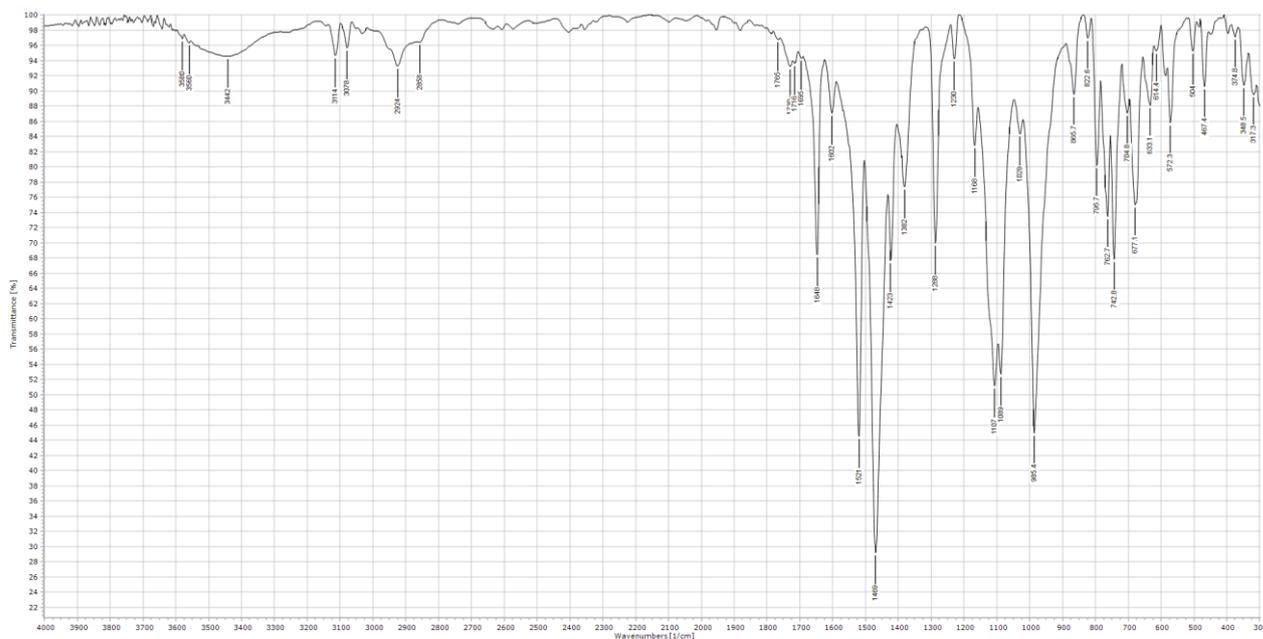

Figure S5 IR spectra of **1** in KBr discs.

Figure S6 IR spectra of **2** in KBr discs.

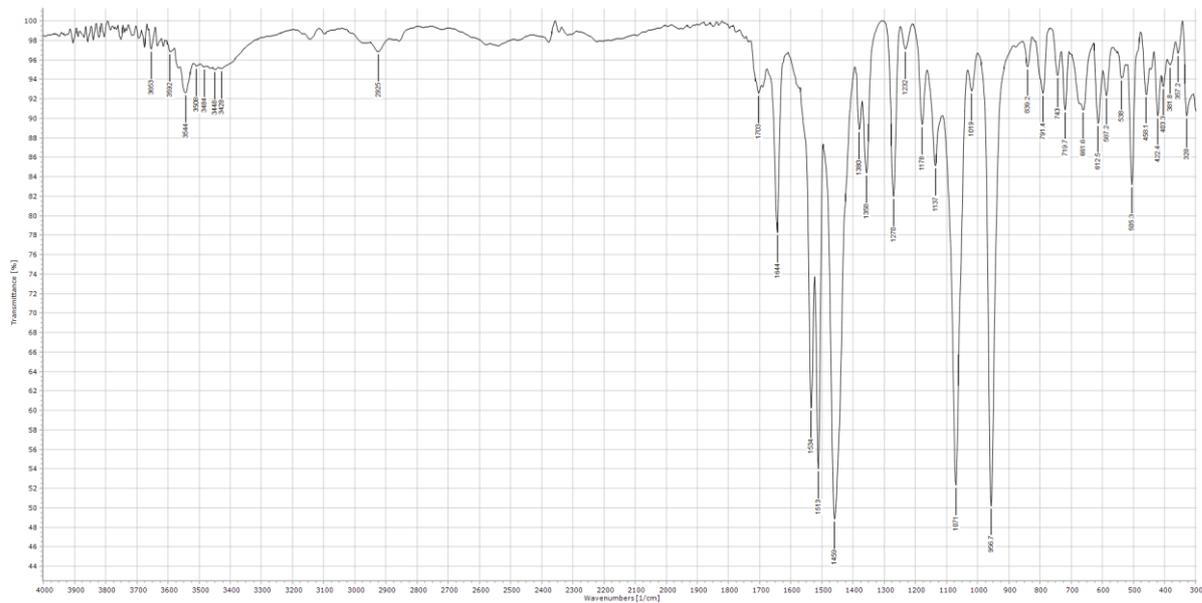**Figure S7** IR spectra of **3** in KBr discs.

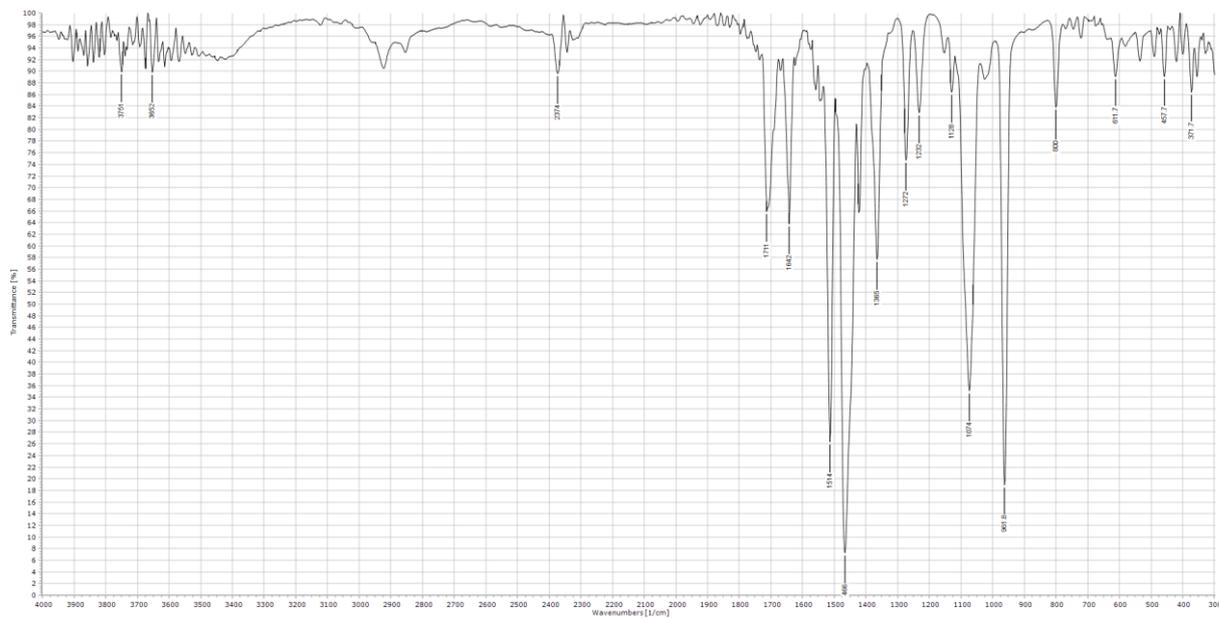**Figure S8** IR spectra of $\{Al(C_6F_5)_3\}_2 \cdot pyz$ in KBr discs.

Figure S9 IR spectra of **4** in KBr discs.
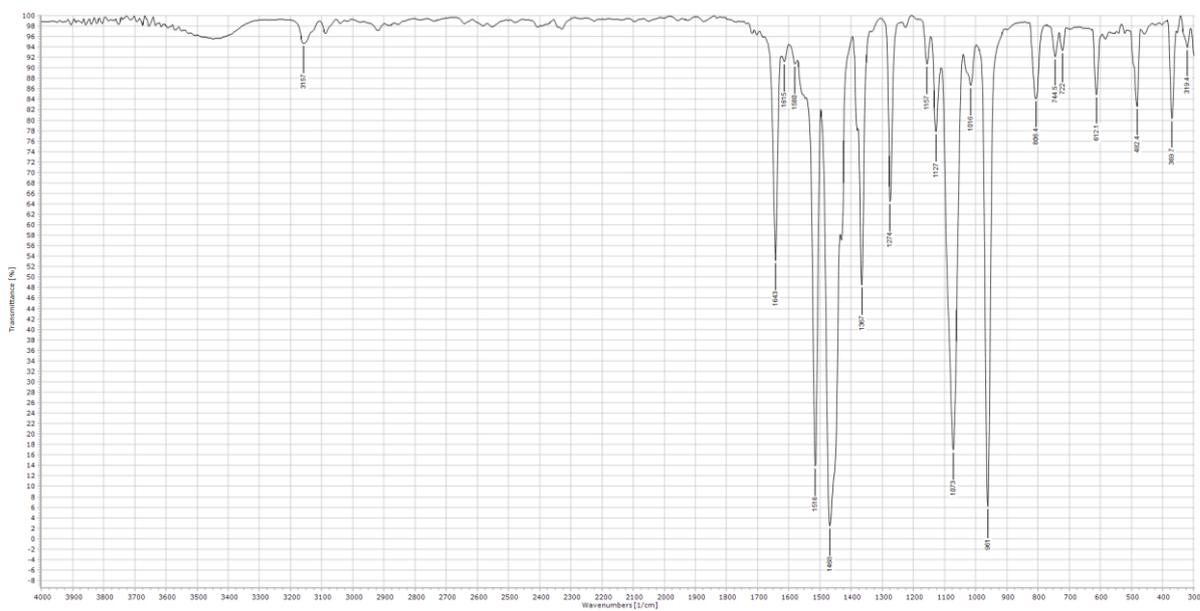
Figure S10 IR spectra of **5** in KBr discs.

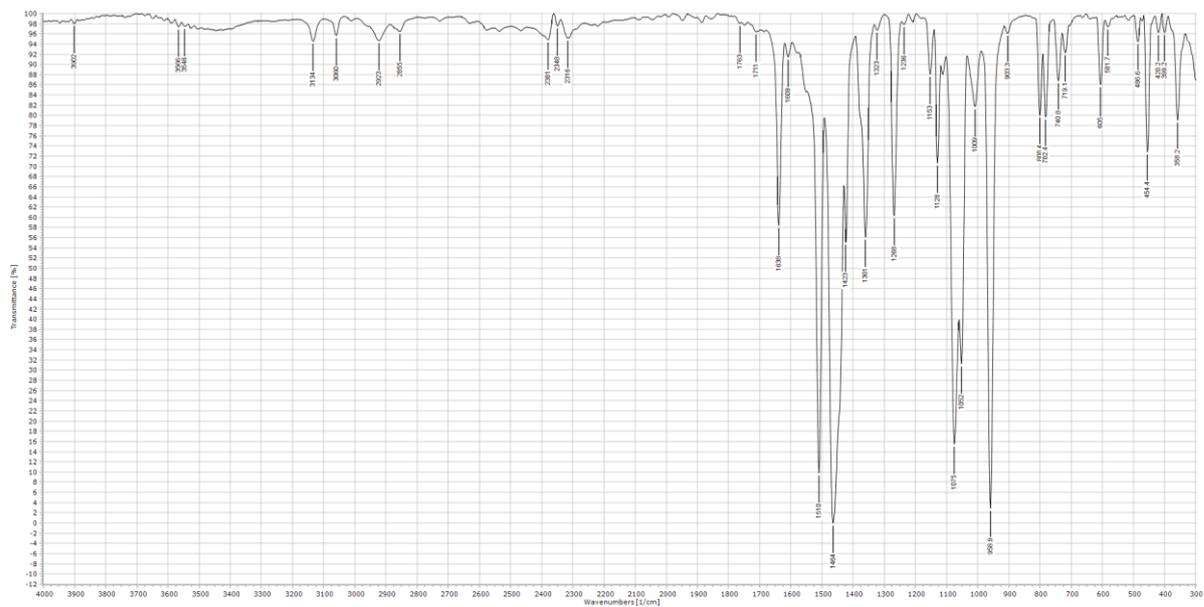**Figure S11** IR spectra in KBr discs of In(C$_6$F$_5$)$_3$·pyz precipitate synthesized by method 1.
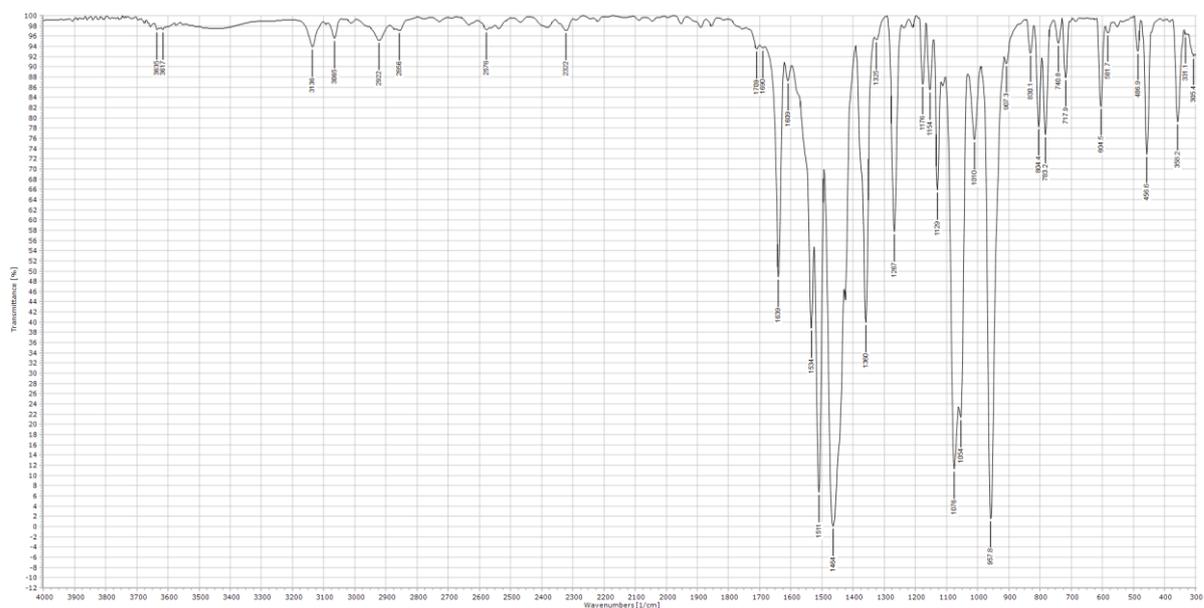
Figure S12 IR spectra in KBr discs of In(C$_6$F$_5$)$_3$·pyz precipitate synthesized by method 2.
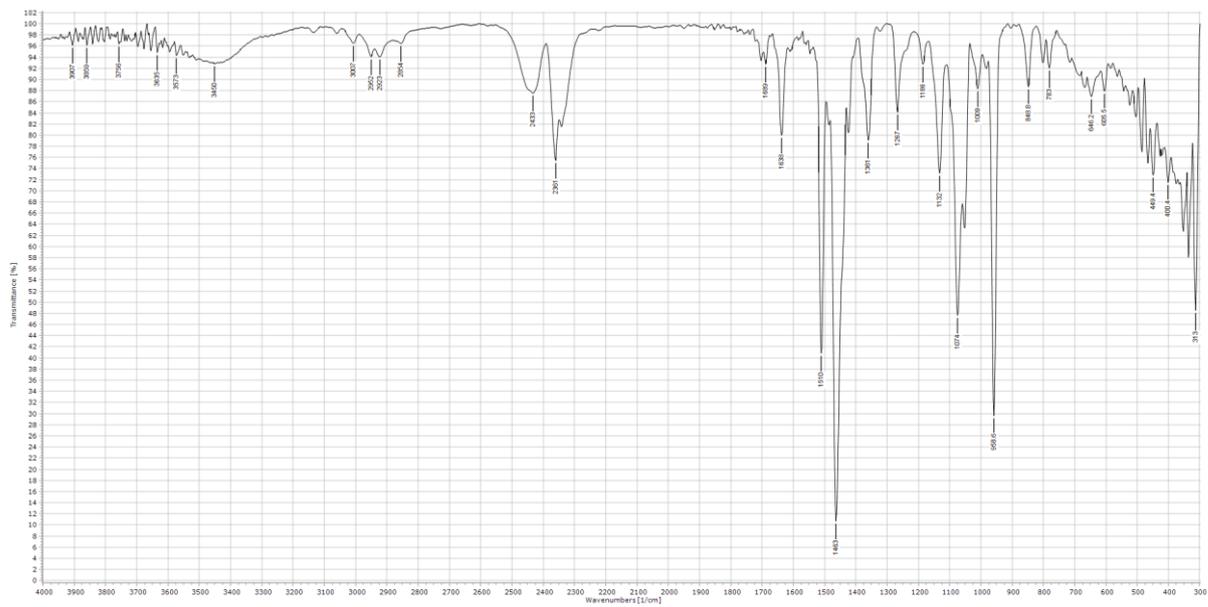
Figure S13 IR spectra of **6** in KBr discs.

Structural studies

For single crystal X-ray diffraction experiment, crystals of **1-6** were fixed on a micro mount and placed on an Agilent Technologies Synergy S using CuK$_\alpha$ monochromated radiation diffractometer. The unit cell parameters were refined by least square techniques. The structure have been solved by the direct methods and refined using SHELXL–97 program[S2] incorporated in the OLEX2 program package[S3]. The hydrogen atoms were placed in calculated positions and were included in the refinement in the 'riding' model approximation, with Uiso(H) set to 1.5Ueq(C). Empirical absorption correction was applied in CrysAlisPro[S4] program complex using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The increased R(int) value of **4** originates from a minor twin component (10%), that was ignored for the refinement. For **7** suitable crystal was selected and placed on Xcalibur, Ruby, Gemini ultra diffractometer. Using Olex2 [S3], the structure was solved with the Superflip[S5-S7] structure solution program using Charge Flipping and refined with the ShelXL[S2] refinement package using Least Squares minimization. Structural data of **1**-**7** were deposited to CCDC database[S8] under deposition numbers 2105697-2105703.

X-ray powder diffraction analysis was performed on a Bruker D2 Phaser instrument with a copper anode.

Figure S14 Molecular structure of **1**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°): B1–N1 1.637(3), B1–C1 1.635(3), B1–C7 1.636(3), B1–C13 1.643(3), N1–B1–C1 111.46(15), N1–B1–C7 104.84(15), N1–B1–C13 100.34(14), C1–B1–C7 104.84(15), C1–B1–C13 116.20(16), C7–B1–C13 114.90(16).

Figure S15 Molecular structure of **2**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°): B1–N1 1.654(3), B2–N2 1.661(3), B1–C1 1.635(4), B1–C7 1.635(4), B1–C13 1.637(4), B2–C23 1.632(4), B2–C29 1.634(4), B2–C35 1.637(4), N1–B1–C1 109.0(2), N1–B1–C7 101.10(19), N1–B1–C13 109.3(2), C1–B1–C7 117.0(2), C1–B1–C13 105.4(2), C7–B1–C13 114.8(2), N2–B2–C23 109.2(2), N2–B2–C29 109.4(2), N2–B2–C35 100.80(19), C23–B2–C29 106.9(2), C23–B2–C35 115.7(2), C29–B2–C35 114.6(2)

Figure S16 Molecular structure of **3**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°): Al1–N1 2.0254(12), Al1–C1   1.9918(14), Al1–C7 1.9936(14), Al1–C13 1.9947(13), N1–Al1–C1 100.94(5), N1–Al1–C7 99.13(5), N1–Al1–C13 104.77(5), C1–Al1–C7 113.64(5), C1–Al1–C13 117.74(6), C7–Al1–C13 116.66(6).
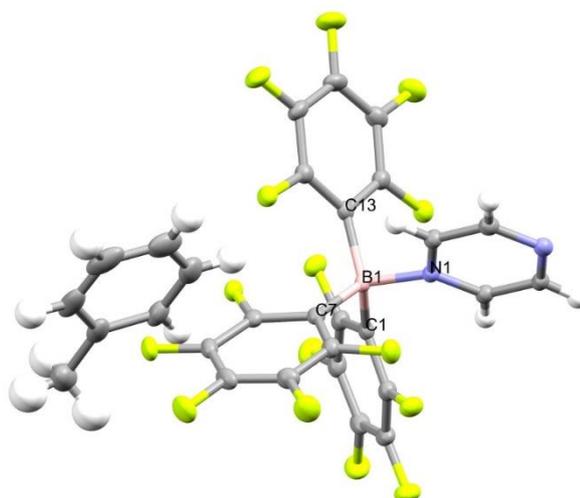
Figure S17 Molecular structure of **4**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°): Ga1–N1 2.097(2), Ga1–C5 1.990(3), Ga1–C11 1.990(3), Ga1–C17 1.986(3), N1–Ga1–C5 98.3(1), N1–Ga1–C11 103.9(1), N1–Ga1–C17 100.3(1), C5–Ga1–C11 117.7(1), C5–Ga1–C17 113.8(1), C11–Ga1–C17 118.0(1).
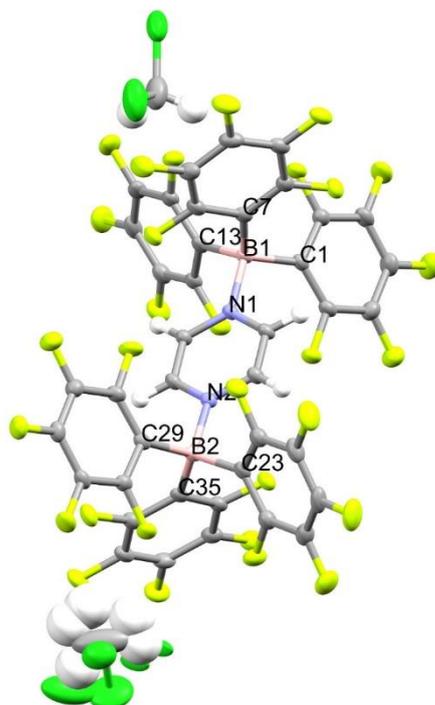

Figure S18 Molecular structure of **5**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°):

Ga1–N1 2.106(2), Ga2–N2 2.122(2), Ga1A–N1A 2.098(2), Ga2A–N2A 2.116(2), Ga1B–N1B 2.091(2), Ga1C–N1C 2.104(2),

Ga1–C1 1.979(3), Ga2–C23 1.985(3), Ga1A–C1A 1.988(3), Ga2A–C23A 1.985(3), Ga1B–C1B 1.980(3), Ga1C–C1C 1.978(3),

Ga1–C7 1.989(3), Ga2–C29 1.988(3), Ga1A–C7A 1.991(3), Ga2A–C29A 1.989(3), Ga1B–C7B 1.981(3), Ga1C–C7C 1.984(3),

Ga1–C13 1.993(3), Ga2–C35 1.990(3), Ga1A–C13A 1.990(3), Ga1A–C35A 1.991(3), Ga1B–C13B 1.981(3), Ga1C–C13C 1.984(3),

N1–Ga1–C1 101.44(10), N2–Ga2–C23 99.11(10), N1A–Ga1A–C1A 104.93(9), N2A–Ga2A–C23A 98.12(10), N1B–Ga1B–C1B 99.50(9), N1C–Ga1C–C1C 104.95(9),

N1–Ga1–C7 100.15(9), N2–Ga2–C29 100.36(10), N1A–Ga1A–C7A 114.77(11), N2A–Ga2A–C29A 102.86(10), N1B–Ga1B–C7B 105.08(9), N1C–Ga1C–C7C 98.51(9),

N1–Ga1–C13 106.43(9), N2–Ga2–C35 103.20(9), N1A–Ga1A–C13A 99.30(9), N2A–Ga2A–C35A 102.83(10), N1B–Ga1B–C13B 102.99(9), N1C–Ga1C–C13C 104.07(10),

C1–Ga1–C7 115.18(11), C23–Ga2–C29 114.00(11), C1A–Ga1A–C7A 114.77(11), C23A–Ga2A–C29A 115.51(11), C1B–Ga1B–C7B 116.18(11), C1C–Ga1C–C7C 115.16(11),

C1–Ga1–C13 115.49(10), C23–Ga2–C35 118.45(11), C1A–Ga1A–C13A 115.81(10), C23A–Ga2A–C35A 114.92(11), C1B–Ga1B–C13B 114.88(11), C1C–Ga1C–C13C 115.93(11),

C7–Ga1–C13 115.28(11), C29–Ga2–C35 117.03(11), C7A–Ga1A–C13A 115.81(10), C29A–Ga2A–C35A 118.31(11), C7B–Ga1B–C13B 115.21(11), C7C–Ga1C–C13C 115.18(11).
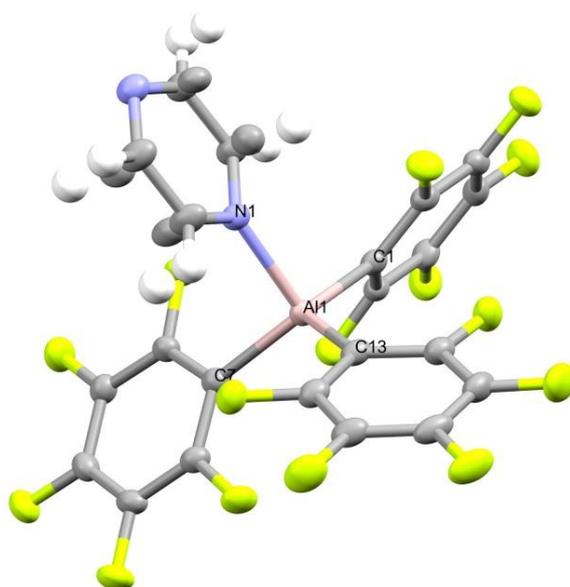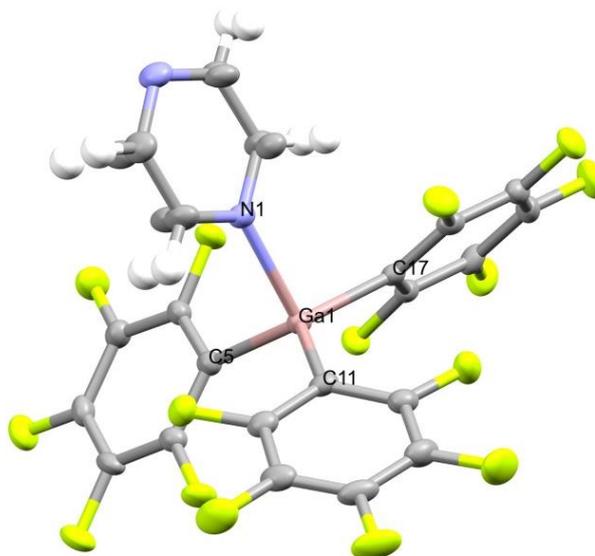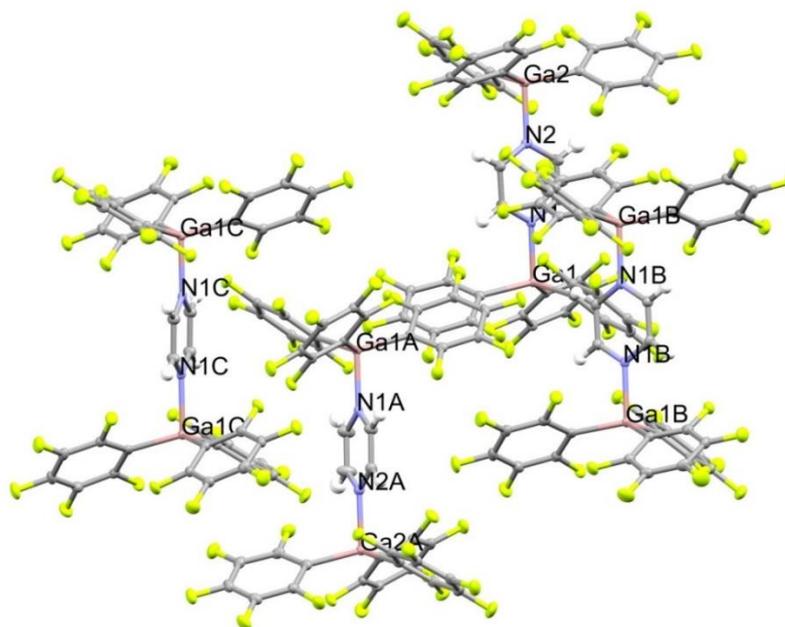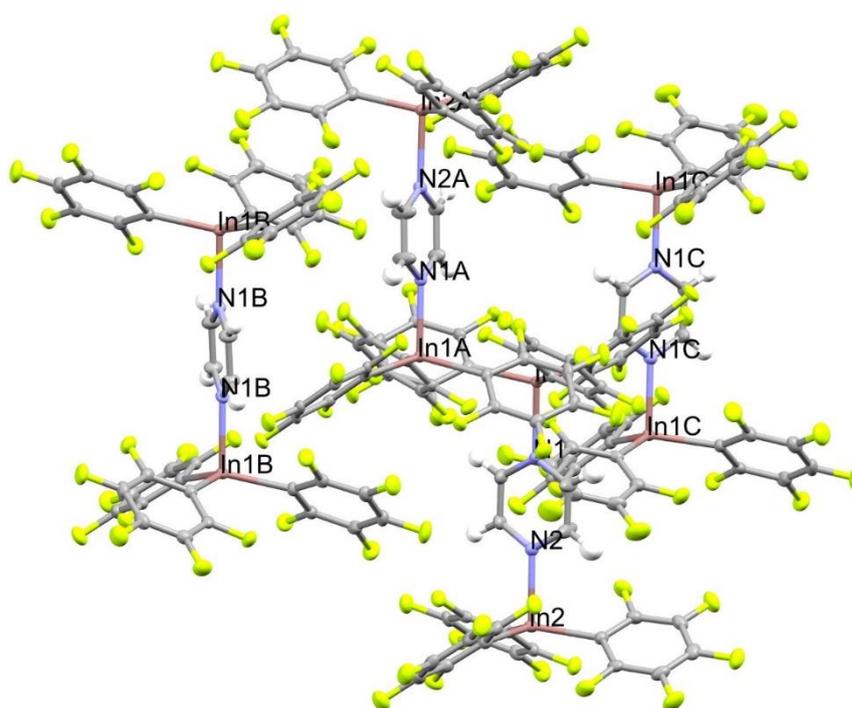

Figure S19 Molecular structure of **6**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°):

In1–N1 2.305(3), In2–N2 2.319(3), In1A–N1A 2.298(3), In2A–N2A 2.322(3), In1B–N1B 2.309(3), In1C–N1C 2.305(3),

In1–C1 2.157(4), In2–C23 2.153(4), In1A–C1A 2.164(4), In2A–C23A 2.160(4), In1B–C1B 2.153(4), In1C–C1C 2.151(4),

In1–C7 2.167(4), In2–C29 2.163(3), In1A–C7A 2.166(3), In2A–C29A 2.161(4), In1B–C7B 2.161(4), In1C–C7C 2.155(4),

In1–C13 2.170(3), In2–C35 2.171(4), In1A–C13A 2.168(4), In2A–C35A 2.164(4), In1B–C13B 2.162(3), In1C–C13C 2.160(4),

N1–In1–C1 99.59(12), N2–In2–C23 97.42(13), N1A–In1A–C1A 102.98(12), N2A–In2A–C23A 100.61(13), N1B–In1B–C1B 102.97(13), N1C–In1C–C1C 97.65(13),

N1–In1–C7 104.68(12), N2–In2–C29 100.50(13), N1A–In1A–C7A 102.43(12), N2A–In2A–C29A 100.44(12), N1B–In1B–C7B 96.98(13), N1C–In1C–C7C 103.69(13),

N1–In1–C13 98.50(12), N2–In2–C35 97.23(12), N1A–In1A–C13A 97.16(12), N2A–In2A–C35A 95.84(12), N1B–In1B–C13B 101.85(12), N1C–In1C–C13C 100.46(13),

C1–In1–C7 116.28(13), C23–In2–C29 118.91(14), C1A–In1A–C7A 115.64(14), C23A–In2A–C29A 120.07(15), C1B–In1B–C7B 115.47(14), C1C–In1C–C7C 117.90(15),

C1–In1–C13 116.45(14), C23–In2–C35 114.09(15), C1A–In1A–C13A 117.69(13), C23A–In2A–C35A 117.32(14), C1B–In1B–C13B 118.13(14), C1C–In1C–C13C 115.24(14),

C7–In1–C13 116.73(14), C29–In2–C35 120.65(14), C7A–In1A–C13A 116.29(14), C29A–In2A–C35A 115.38(15), C7B–In1B–C13B 116.40(14), C7C–In1C–C13C 116.89(14).
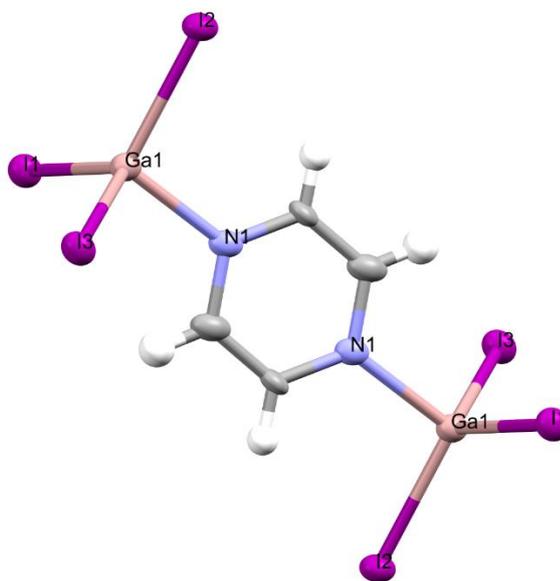

Figure S20 Molecular structure of **7**. Ellipsoids at 50% probability level. Selected bond lengths (Å) and valence angles (°): Ga1–N1 2.092(6), Ga1–I1 2.4864(8), Ga1–I2 2.5279(9), Ga1–I3 2.5087(9), N1–Ga1–I1 100.68(14), N1–Ga1–I2 103.11(16), N1–Ga1–I3 101.94(15), I1–Ga1–I2 117.80(3), I1–Ga1–I3 115.65(3), I2–Ga1–I3 114.13(3).

Table S1 Crystal data and structure determination parameters for **1**-**7**.

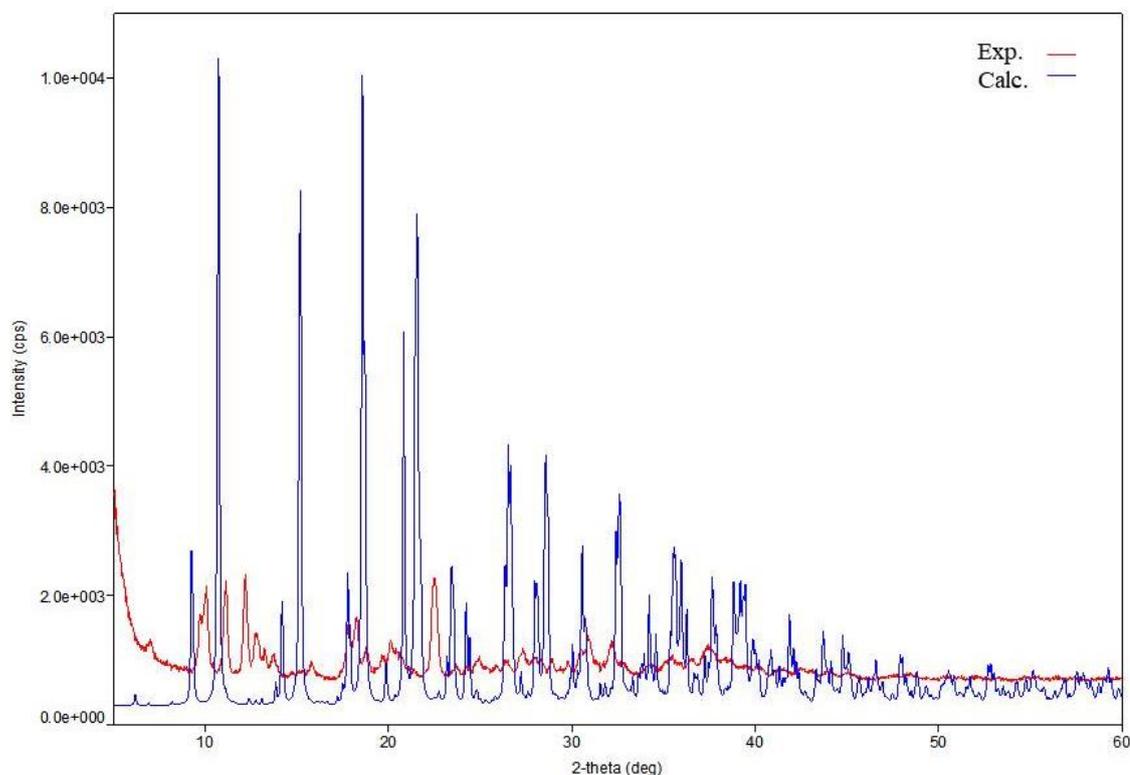| Compound	**1**·Toluene	**2**·2CH$_2$Cl$_2$	**3**	**4**	**5**	**6**	**7**
Formula	C$_{29}$H$_{12}$BF$_{15}$N$_2$	C$_{42}$H$_8$B$_2$Cl$_4$F$_{30}$N$_2$	C$_{22}$H$_4$AlF$_{15}$N$_2$	C$_{22}$H$_4$F$_{15}$GaN$_2$	C$_{40}$H$_4$F$_{30}$Ga$_2$N$_2$	C$_{40}$H$_4$F$_{30}$In$_2$N$_2$	C$_4$H$_4$Ga$_2$I$_6$N$_2$
Mr	684.21	1273.91	608.24	650.98	1221.87	1312.06	980.93
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	triclinic	triclinic
Space group	Cc	P2$_1$/n	P2$_1$/c	P2$_1$/c	P$\bar{1}$	P$\bar{1}$	P$\bar{1}$
a /Å	14.3783(1)	14.1392(1)	12.6505(1)	12.5970(2)	12.6496(1)	12.78749(8)	6.4268(4)
b /Å	11.0646(1)	15.8913(2)	8.0408(1)	8.1516(1)	16.2893(1)	16.56864(9)	7.3619(4)
c /Å	16.7682(1)	19.9879(2)	21.2853(2)	21.2344(4)	28.0758(2)	28.47470(16)	9.7451(7)
α /°	90	90	90	90	89.907(1)	90.0894(4)	81.465(5)
β /°	96.031(1)	100.099(1)	96.201(1)	96.133(2)	89.156(1)	90.5622(5)	84.767(6)
γ /°	90	90	90	90	89.953(1)	90.1349(5)	69.644(5)
V /Å^3	2652.89(3)	4421.50(8)	2152.49(4)	2167.99(6)	5784.47(7)	6032.66(6)	427.11(5)
Z	4	4	4	4	6	6	1
Temperature/K	100.0(3)	99.9(8)	99.9(3)	100.0(2)	100.0(2)	99.96(14)	123.05(10)
Reflections	36201	76953	17013	25345	81534	93995	4498
Ind. reflections	5151	8398	4376	4401	19660	21820	1736
R$_{int}$	0.0352	0.0481	0.0347	0.0846	0.0380	0.0452	0.0457
R$_1$ / wR$_2$ [I>=2σ (I)]	0.0218 / 0.0577	0.0515 / 0.1340	0.0286 / 0.0766	0.0503 / 0.1367	0.0341 / 0.0913	0.0331 / 0.0830	0.0333 / 0.0741
R$_1$ / wR$_2$ [all data]	0.0222 / 0.0580	0.0558 / 0.1373	0.0318 / 0.0788	0.0528 / 0.1385	0.0381 / 0.0935	0.0351 / 0.0839	0.0423 / 0.0766
μ/mm^{-1}	1.579	3.990	2.233	3.134	3.450	10.830	13.970

Figure S21 XRD of $In(C_6F_5)_3 \cdot pyz$ precipitate from the reaction of $In(C_6F_5)_3 \cdot Et_2O$ and pyz (red); calculated values from the crystal structure of **6** (blue).

Mass spectrometric study

Mass-spectrometry studies were performed on Thermoscientific ISQ quadruple mass-spectrometer with Direct Insertion Probe (DIP) equipment (electron ionization, 70 eV, m/Z range 15—1100 amu, measurement rate 5 spectra per second). A sample (0.5-1 mg) was placed in thin glass ampoule (10 mm length and 1 mm diameter) in argon-filled glove box. Ampoules were opened on air and immediately placed into DIP. Gaseous products were directly injected into ionization chamber. Pressure in the ionization chamber during experiment was 10^{-4}-10^{-5} torr. Mass-spectra of the gas phase above **1-5** were measured from 313 K to 573 K with 10 K/min heating rate.

At 400-470 K ion $C_7H_8^+$ observed as a result of toluene loss from **1**. At 400-470 K the most intensive ion in mass-spectrum above **1** is Pyz^+. At 460 K $B(C_6F_5)_3^+$ (34%) and $B(C_6F_5)_3Pyz^+$ (5%) also observed. At temperatures above 470-500 K the most intensive ion in mass-spectrum above **1** is $B(C_6F_5)_3^+$ (100%), while intensity of Pyz^+ decrease with further heating. Intensity of $B(C_6F_5)_3Pyz^+$ ion is small ($\leq 5\%$), that indicates preliminary dissociation over evaporation during heating **1**. In mass-spectrum above **2** $CH_2Cl_2^+$ ion is observed in temperature range 350-430 K as a result of dichloromethane loss. An ions Pyz^+, $B(C_6F_5)_3^+$ appeared at 370-520 K. $B(C_6F_5)_3Pyz^+$ ion with low ($\leq 2\%$) presented in mass-spectra above **2** at 500-520 K. Intensities of $B(C_6F_5)_3^+$ and Pyz^+ as a function of temperature in mass-spectra above **1** (Fig. 23S) and **2** (Fig. 25S) can be explained by dissociation of $B(C_6F_5)_3Pyz$ with pyrazine elimination and $[B(C_6F_5)_3]_2Pyz$ formation with further dissociation to donor and acceptor. Heating both **3** and **4** result in pyrazine and pentafluorobenzene formation in temperature range 320-480 K as a main gaseous products. Ions $Al(C_6F_5)_3^+$ and $Al(C_6F_5)_3Pyz^+$ observed at 540-570 K with low intensities ($\leq 0.3\%$). At 540-570 K

in gas phase under **3** an ions AlF_2Pyz^+, $Al(C_6F_5)F_2^+$, $Al(C_6F_5)_2F^+$, $Al(C_6F_5)FPyz^+$ with significant higher relative intensities than $Al(C_6F_5)_3^+$ and $Al(C_6F_5)_3Pyz^+$ (Fiq 27S). Thus, for **3** and $\{Al(C_6F_5)_3\}_2 \cdot pyz$ thermal decomposition precedes vaporization of the complexes. At 350-470 K the most intensive ion in mass-spectrum above **4** is Pyz^+. Low intensities of gallium-containing ions at 350-470 K observed. An ions $Ga(C_6F_5)_3^+$ and $Ga(C_6F_5)_3Pyz^+$ appeared at 450 K and 510 K respectively. In mass-spectrum above **5** increasing intensities of $Ga(C_6F_5)_3^+$ and Pyz^+ is observed in temperature range 450-570 K as a result of dissociation process. In mass-spectrum of gas phase above **4** and **5** an $C_6F_5H^+$ ion observed at temperatures above 350 K as a result of thermal decomposition with pentafluorobenzene formation. Intensities of $Ga(C_6F_5)_3^+$ and Pyz^+ as a function of temperature in mass-spectra above **4** (Fig. 31S) and **5** (Fig. 33S) can be explained by dissociation of $Ga(C_6F_5)_3Pyz$ with pyrazine elimination and $[Ga(C_6F_5)_3]_2Pyz$ formation with further dissociation to donor and acceptor. Mass-spectra for samples, prepared by reaction of $In(C_6F_5)_3Et_2O$ with pyrazine with 1:1 and 2:1 ratios, are similar. At 370-380 K an ion Pyz^+ appears without significant In-containing ions observed (Fig. 35S, 37S). Further heating lead to intensity increase of Pyz^+ and $In(C_6F_5)_3^+$, $In(C_6F_5)_2Pyz^+$ that indicate evaporation and dissociation of complex. In mass-spectra under **6** an ions Pyz^+ and $C_6F_5H^+$ observed with comparable intensities, that differs from mass-spectra of precipitates after reaction of $In(C_6F_5)_3Et_2O$ with pyrazine with 1:1 and 2:1 ratios. $In(C_6F_5)_3^+$, $In(C_6F_5)_2Pyz^+$ appeared at 500 K as a result of evaporation and dissociation of complex. It should be noted, that in mass-spectra above **1-5** an $C_6F_5H^+$ ion observed as a result of partial thermal decomposition with pentafluorobenzene formation.

Figure S22 Mass-spectra of the gas phase above **1** at 460 K.

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Figure S23 Relative intensity of selected ions in mass-spectra of the gas phase above **1** as a function of temperature. 1 - $C_7H_8^+$, 2 - Pyz^+, 3 - $C_6F_5H^+$, 4 - $B(C_6F_5)_3^+$, 5 - $B(C_6F_5)_3Pyz^+$.

Figure S24 Mass-spectra of the gas phase above **2** at 460 K.

Figure S25 Relative intensity of selected ions in mass-spectra of the gas phase above **2** as a function of temperature. $1 – CH_2Cl_2^+$, $2 - Pyz^+$, $3 - C_6F_5H^+$, $4 - B(C_6F_5)_3^+$, $5 - B(C_6F_5)_3Pyz^+$.

Figure S26 Mass-spectra of the gas phase above **3** at 570 K.

Figure S27 Relative intensity of selected ions in mass-spectra of the gas phase above **3** as a function of temperature. 1 - Pyz^+, 2 - $C_6F_5H^+$, 3 - $Al(C_6F_5)_3^+$, 4 - $Al(C_6F_5)_3Pyz^+$, 5 - AlF_2Pyz^+, 6 - $Al(C_6F_5)F_2^+$, 7 - $Al(C_6F_5)_2F^+$, 8 - $Al(C_6F_5)FPyz^+$.
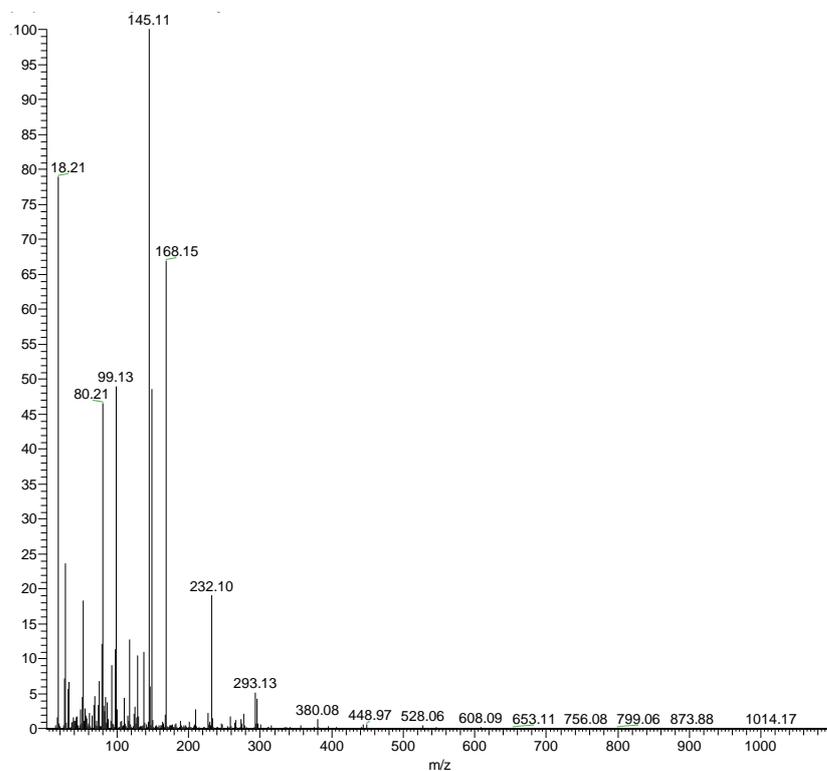
Figure S28 Mass-spectra of the gas phase above $\{Al(C_6F_5)_3\}_2 \cdot pyz$ at 570 K.
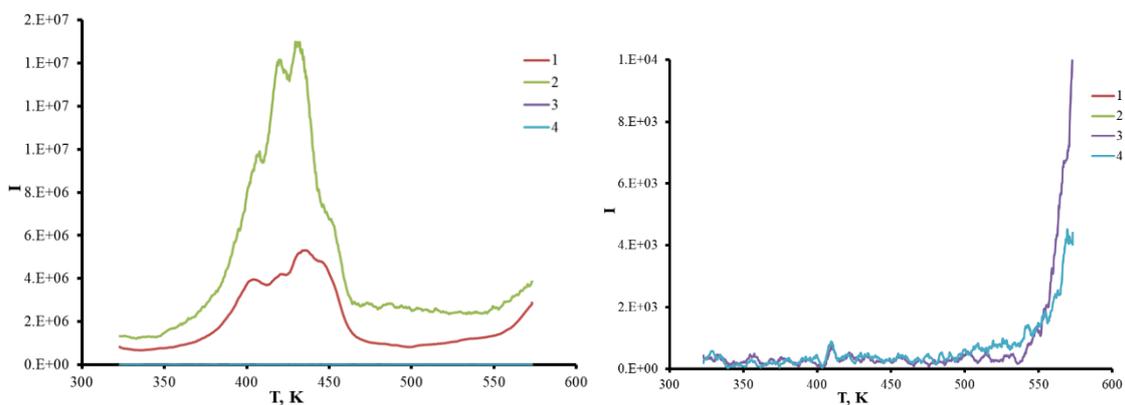
Figure S29 Relative intensity of selected ions in mass-spectra of the gas phase above $\{Al(C_6F_5)_3\}_2 \cdot pyz$ as a function of temperature. 1 - Pyz^+, 2 - $C_6F_5H^+$, 3 - $Al(C_6F_5)_3^+$, 4 - $Al(C_6F_5)_3Pyz^+$.

Figure S30 Mass-spectra of the gas phase above **4** at 570 K.

Figure S31 Relative intensity of selected ions in mass-spectra of the gas phase above **4** as a function of temperature. 1 - Pyz^+, 2 - $C_6F_5H^+$, 3 - $Ga(C_6F_5)_3^+$, 4 - $Ga(C_6F_5)_3Pyz^+$.

Figure S32 Mass-spectra of the gas phase above **5** at 570 K.

Figure S33 Relative intensity of selected ions in mass-spectra of the gas phase above **5** as a function of temperature. 1 - Pyz^+, 2 - $C_6F_5H^+$, 3 - $Ga(C_6F_5)_3^+$, 4 - $Ga(C_6F_5)_3Pyz^+$.
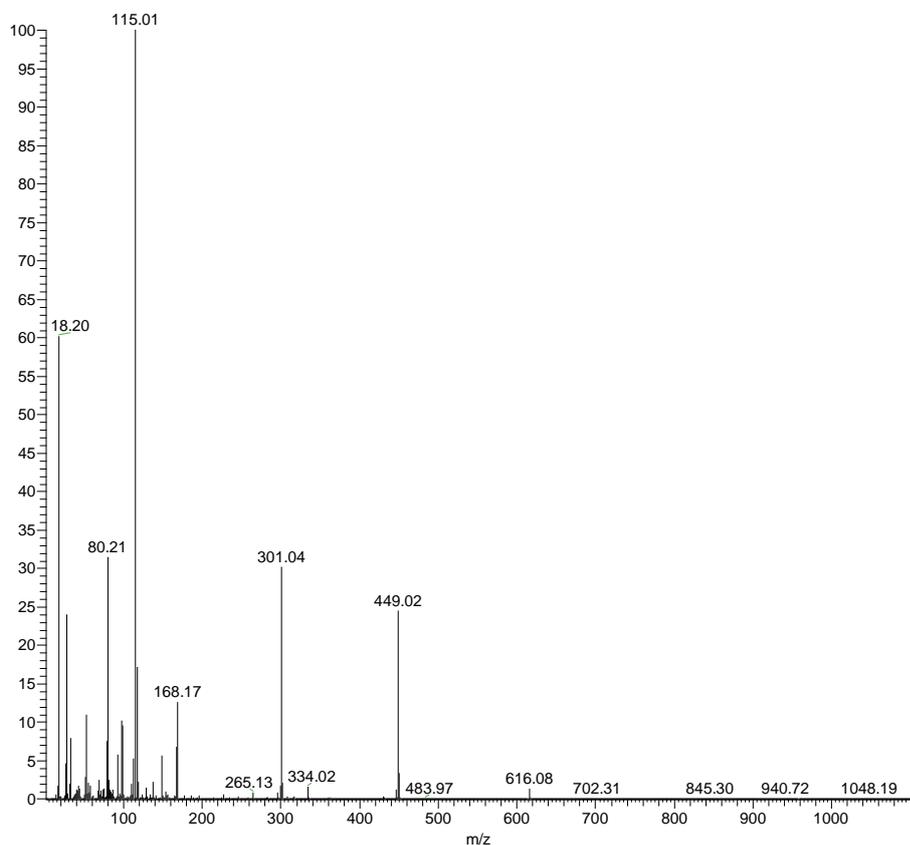
Figure S34 Mass-spectra at 550 K of the gas phase above In(C$_6$F$_5$)$_3$pyz precipitate obtained by method 1.
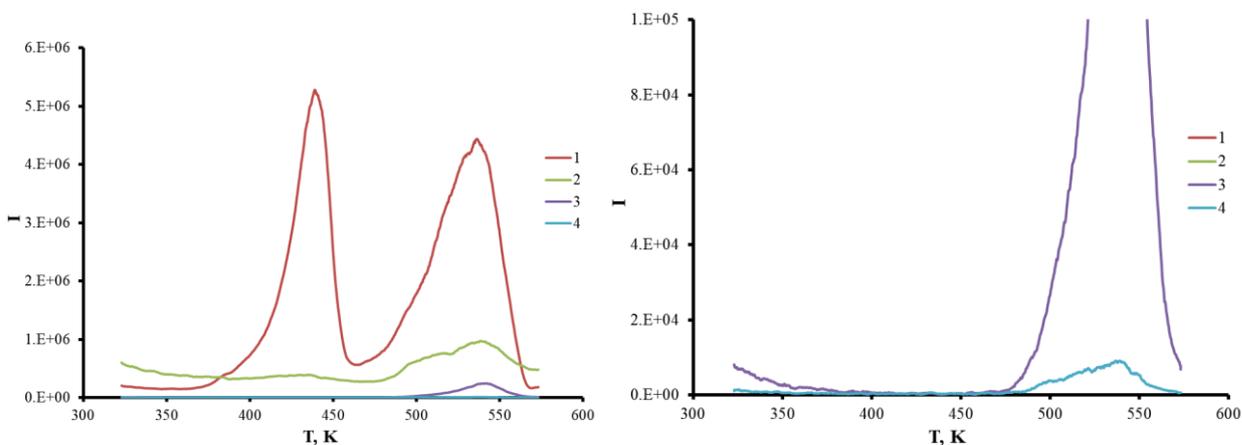
Figure S35 Relative intensity of selected ions in mass-spectra of the gas phase above In(C$_6$F$_5$)$_3$pyz precipitate obtained by method 1 as a function of temperature. 1 - Pyz$^+$, 2 - C$_6$F$_5$H$^+$, 3 - In(C$_6$F$_5$)$_3$$^+$, 4 - In(C$_6F_5$)$_2Pyz^+$.
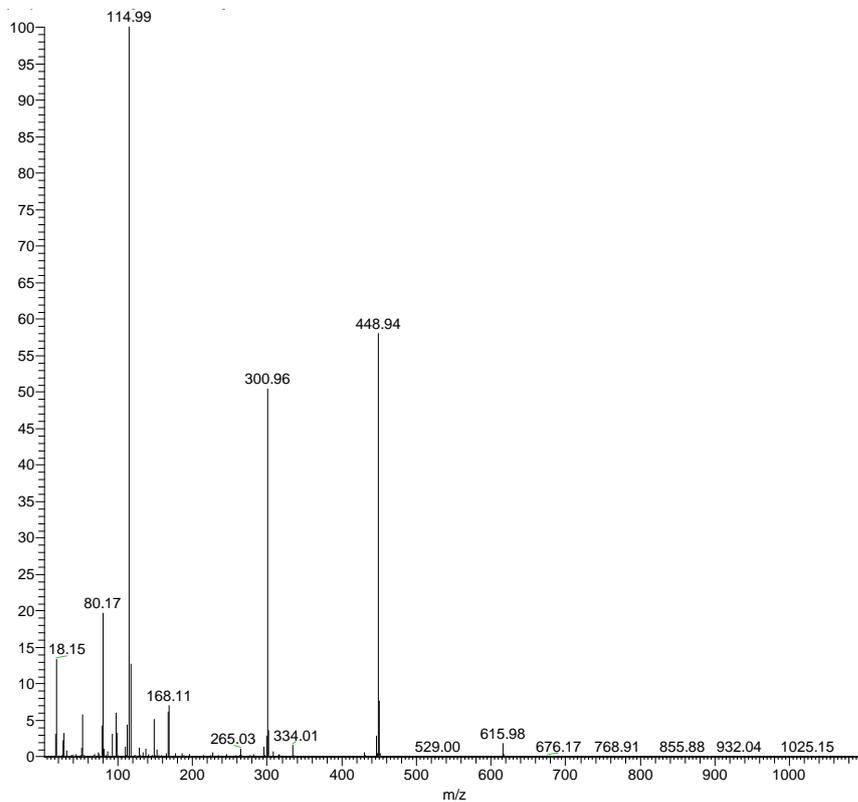
Figure S36 Mass-spectra of the gas phase above In(C$_6$F$_5$)$_3$pyz precipitate obtained by method 2 at 550 K.
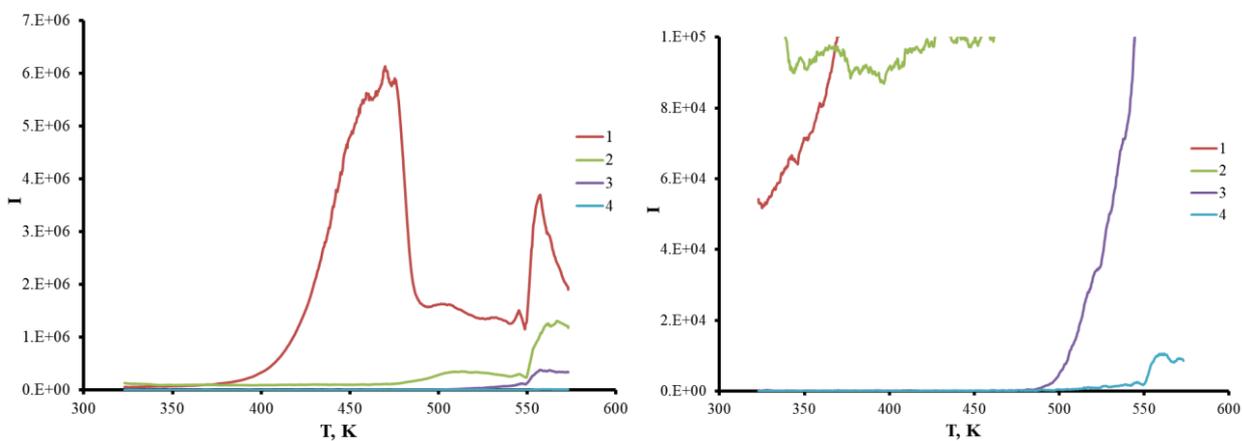
Figure S37 Relative intensity of selected ions in mass-spectra of the gas phase above In(C$_6$F$_5$)$_3$pyz precipitate obtained by method 2 as a function of temperature. 1 - Pyz$^+$, 2 - C$_6$F$_5$H$^+$, 3 - In(C$_6$F$_5$)$_3^+$, 4 - In(C$_6$F$_5$)$_2$Pyz$^+$.
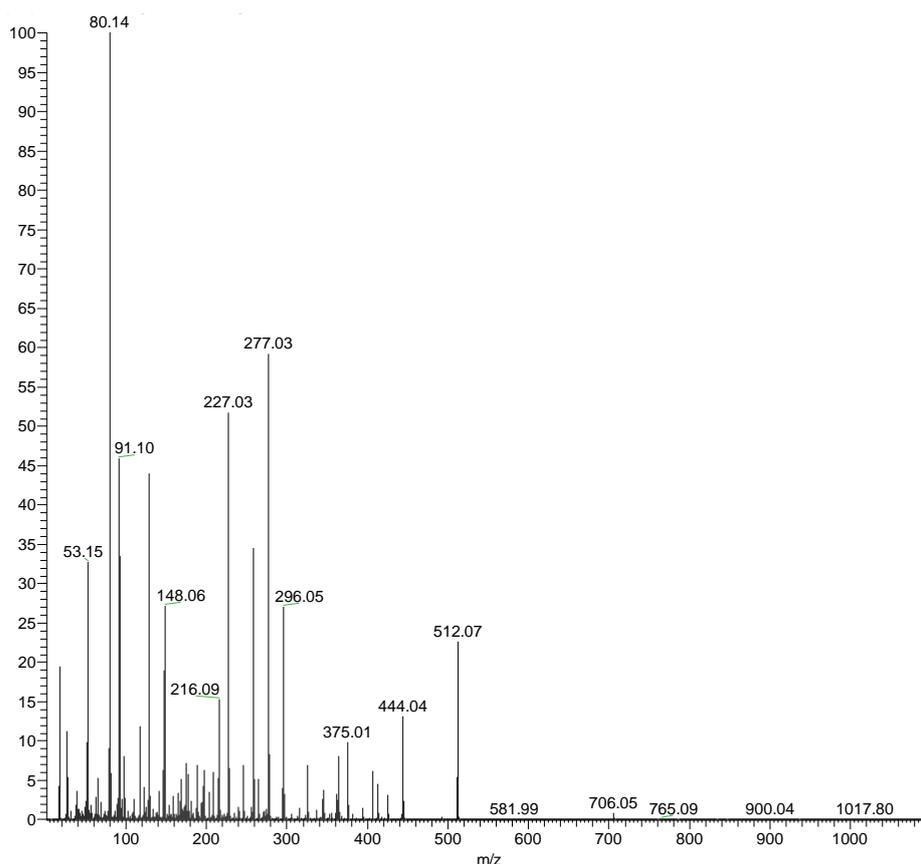
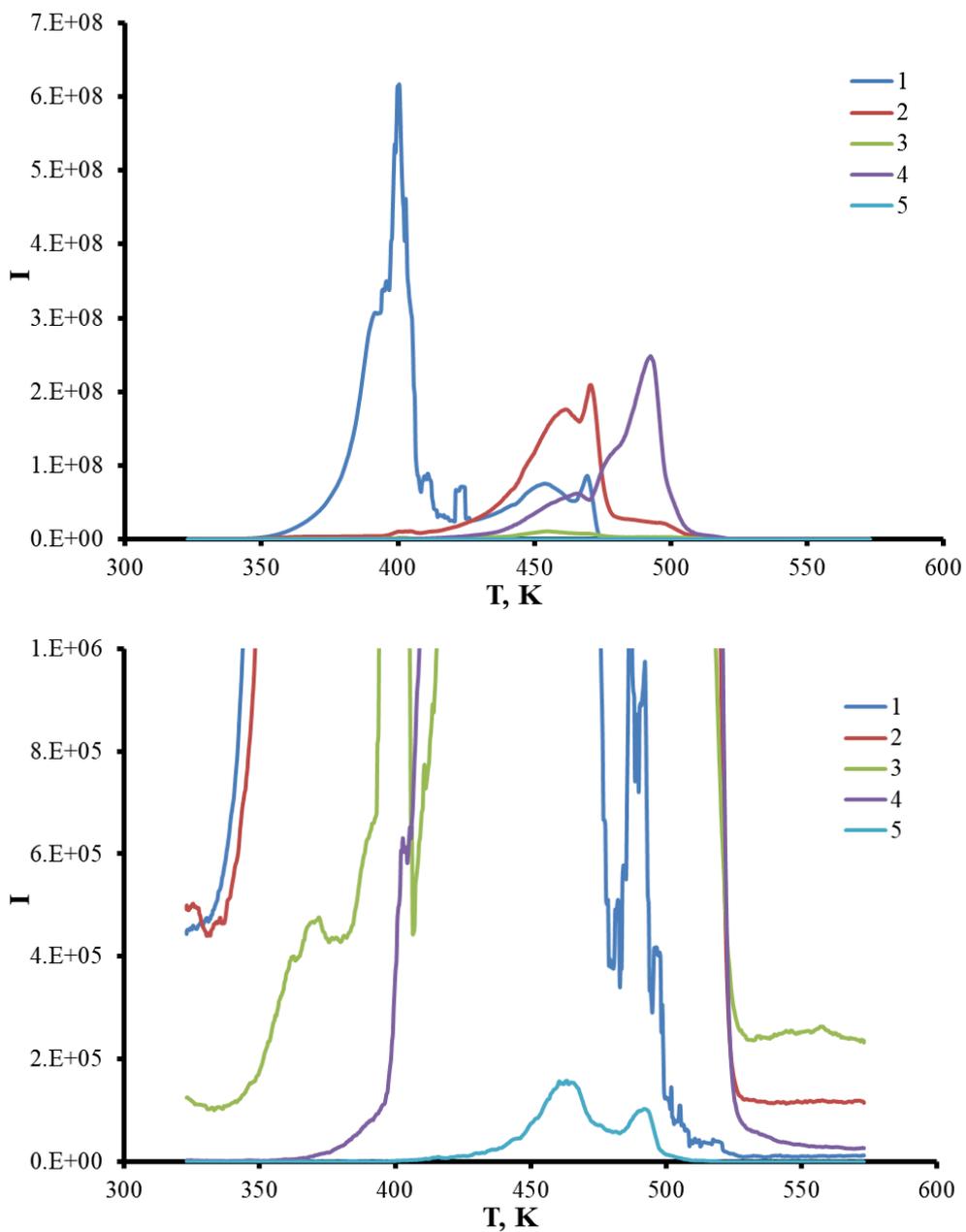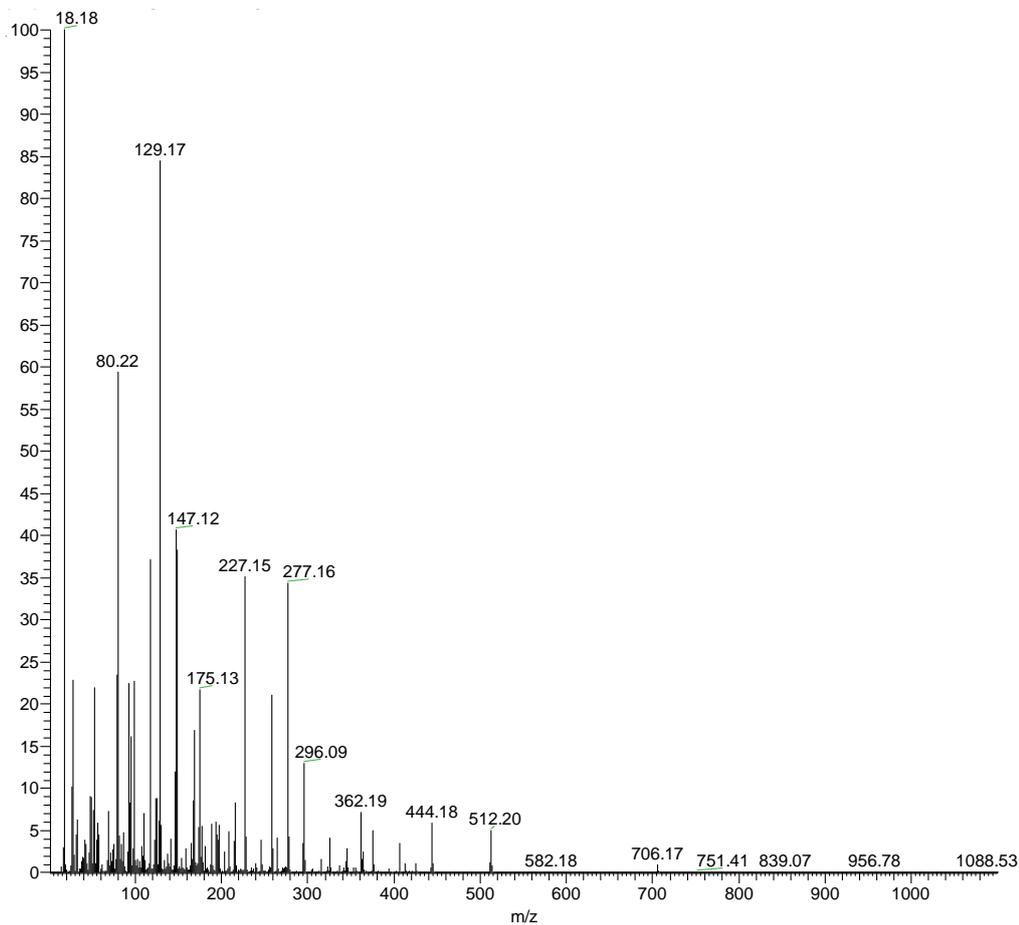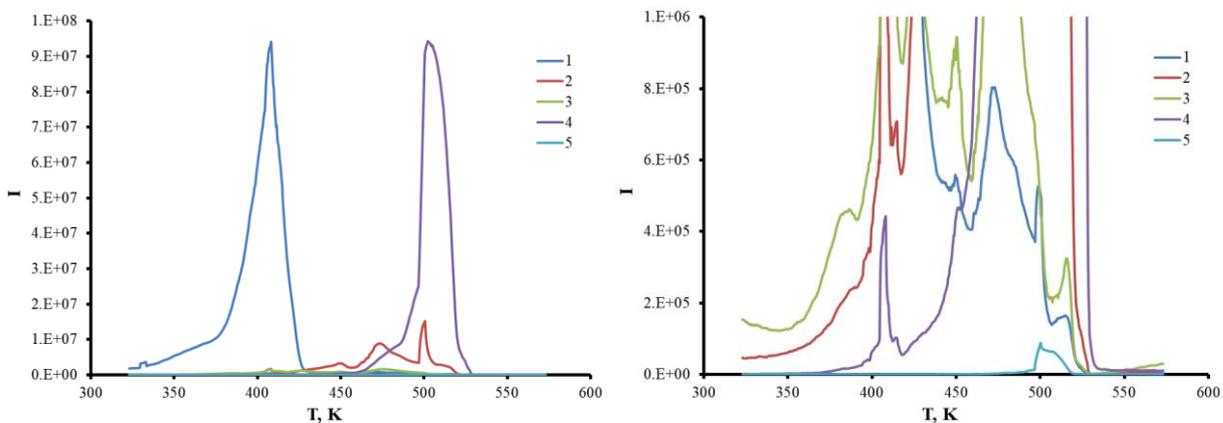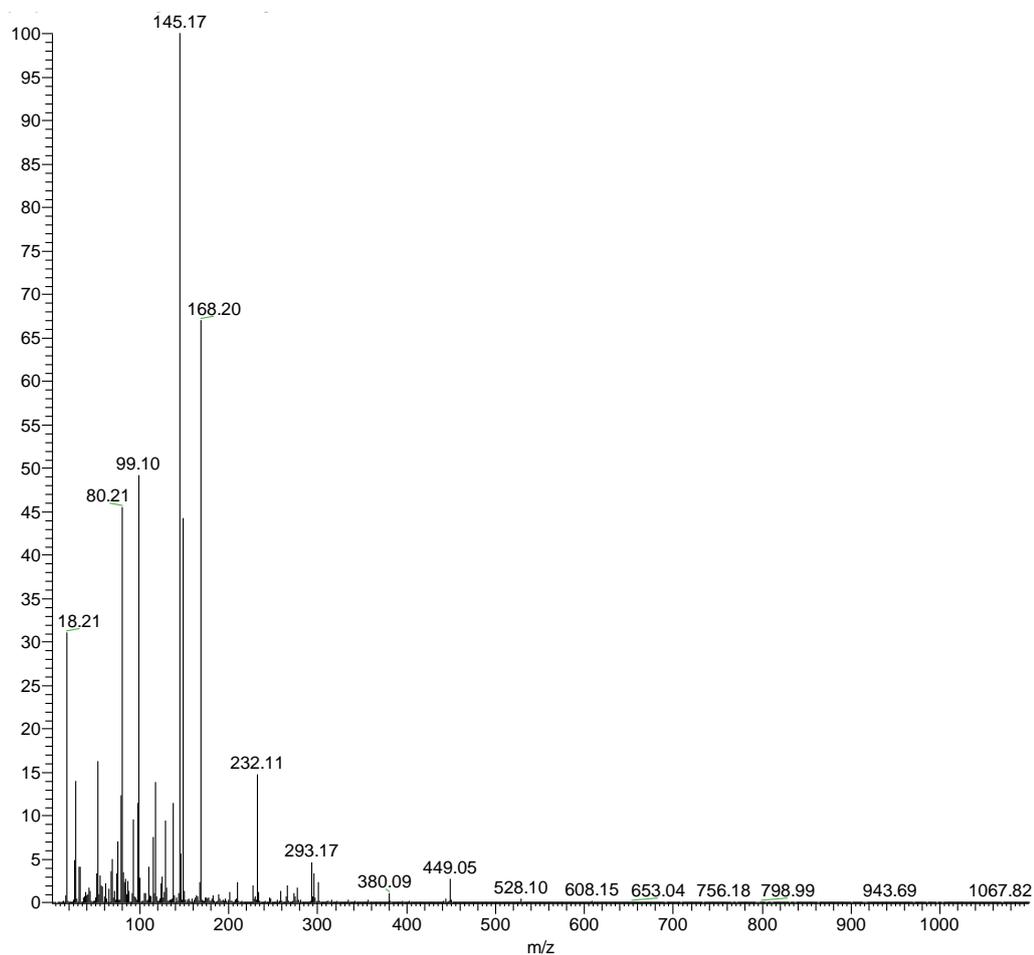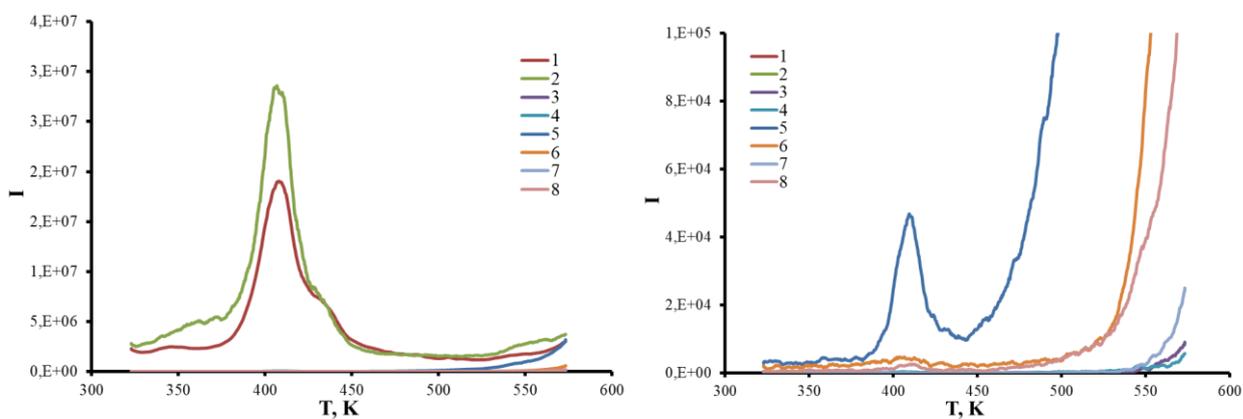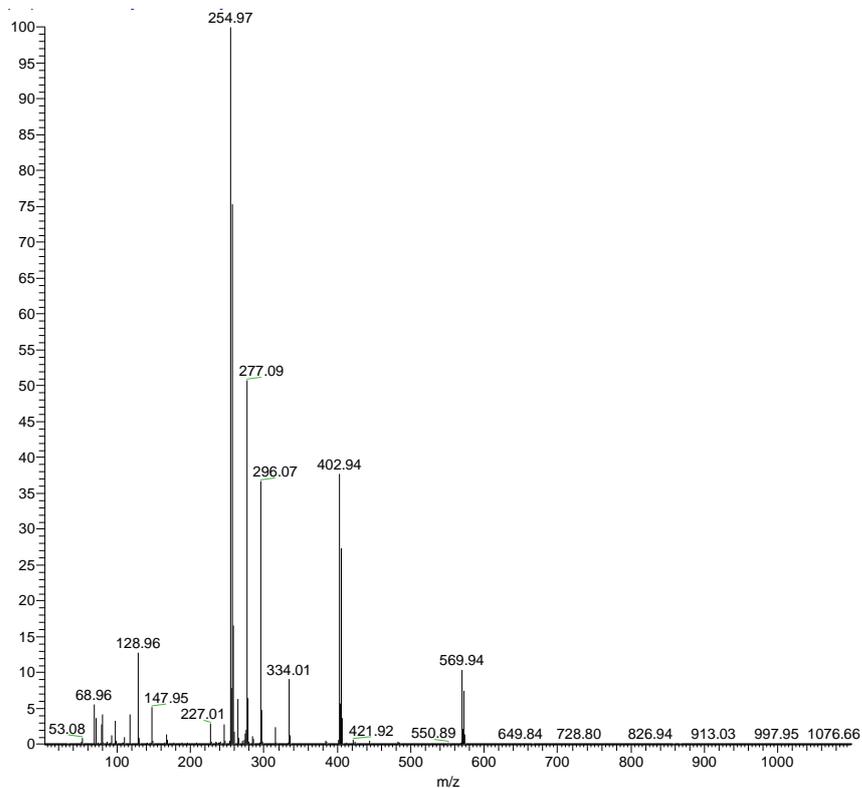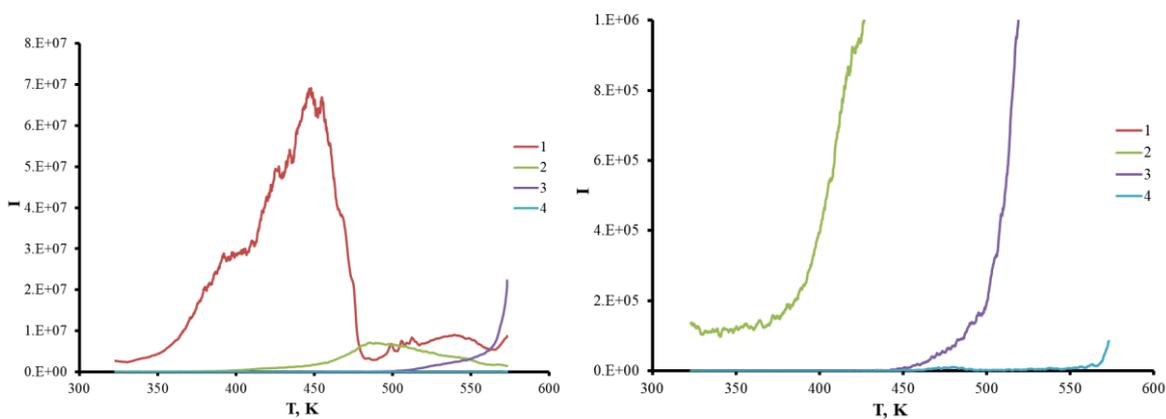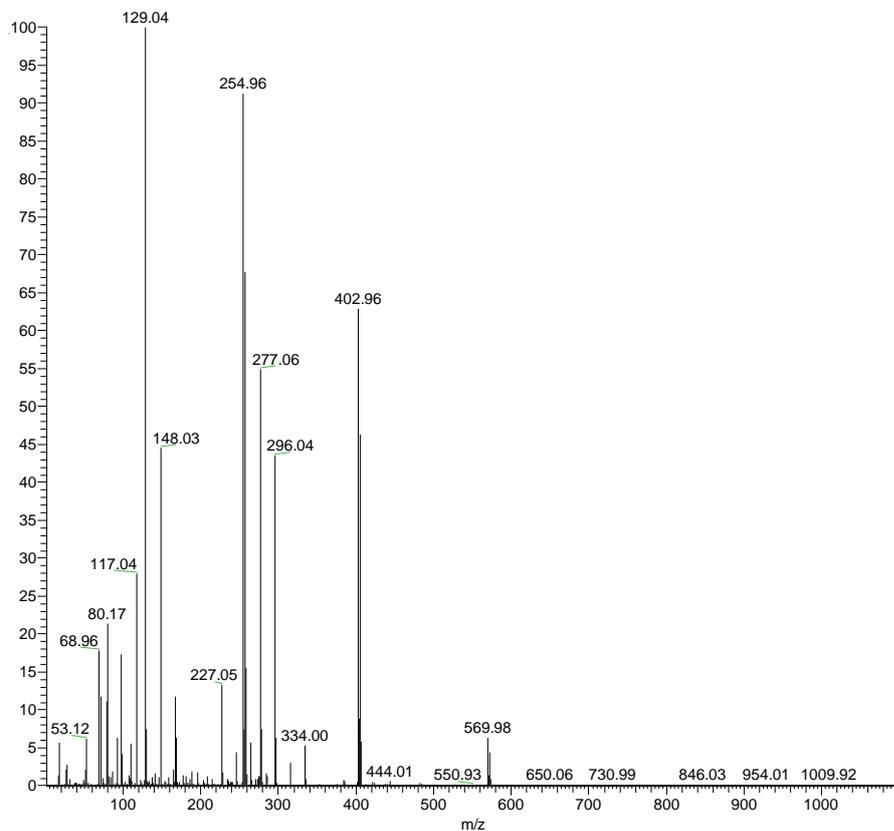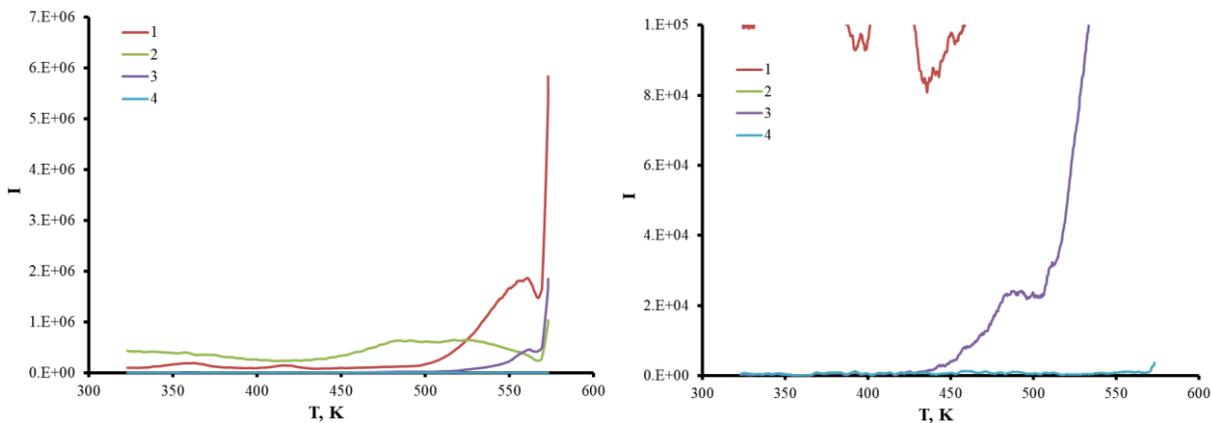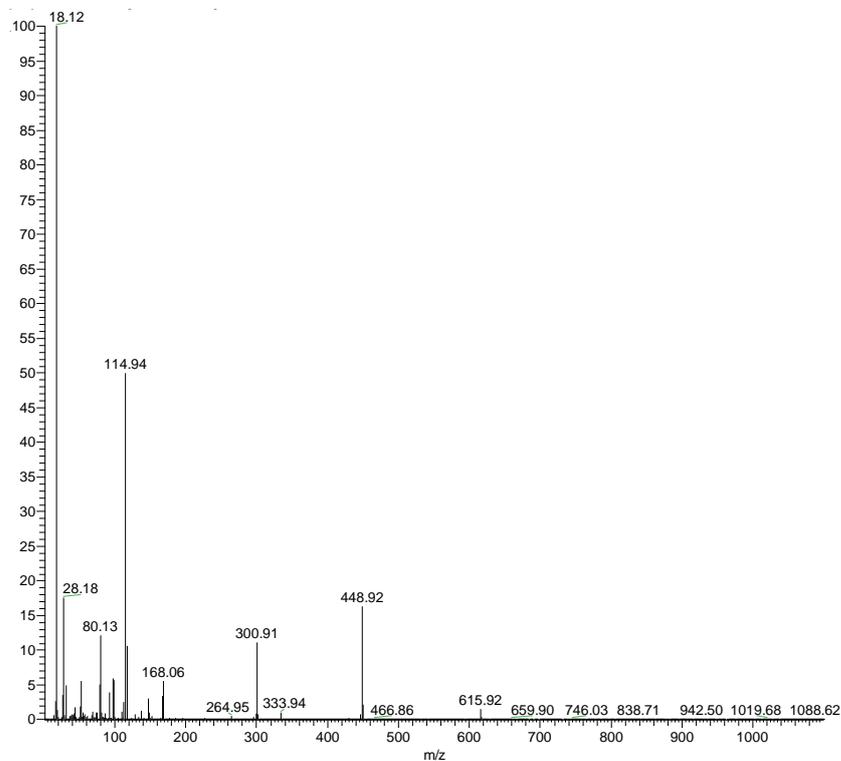**Figure S38** Mass-spectra of the gas phase above **6** at 550 K.
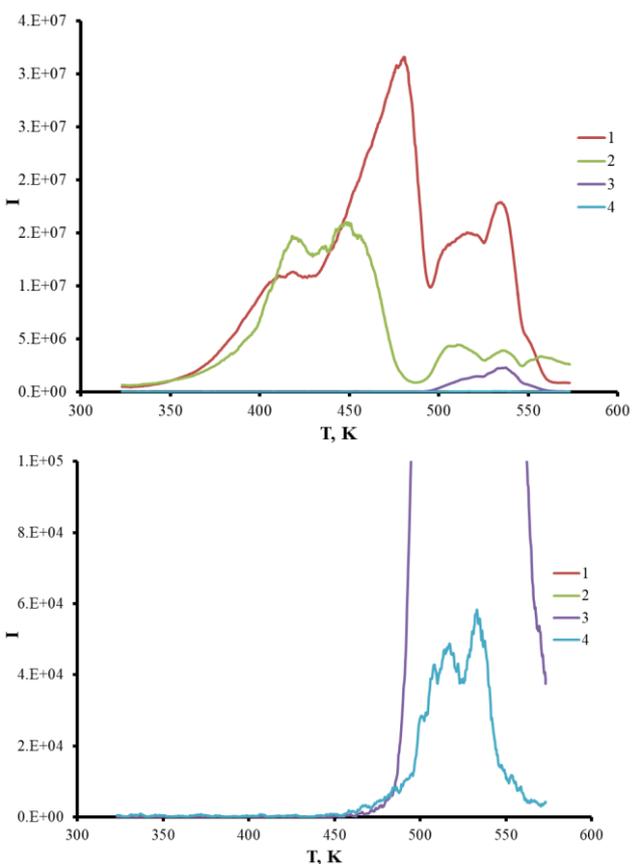
Figure S39 Relative intensity of selected ions in mass-spectra of the gas phase above 6 as a function of temperature. 1 - Pyz^+, 2 - $C_6F_5H^+$, 3 - $In(C_6F_5)_3^+$, 4 - $In(C_6F_5)_2Pyz^+$.

Computational data.

Table S2 Thermodynamic characteristics for the gas phase dissociation processes of studied complexes with pyrazine. Standard reaction enthalpies $\Delta_{diss}H°_{298}$, reorganization energies $\Delta_{reorg}E_{LA}$ and donor-acceptor bond energies E_{DA} in kJ mol^{-1}, standard reaction entropies $\Delta_{diss}S°_{298}$ in J mol^{-1} K^{-1}. M06-2X/def2-TZVP level of theory.

Reaction	$\Delta_{diss}H°_{298}$	$\Delta_{diss}S°_{298}$	$\Delta_{reorg}E_{LA}$	E_{DA}
$B(C_6F_5)_3 \cdot pyz = B(C_6F_5)_3 + pyz$	106.6	187.5	118.5	235.5
$Al(C_6F_5)_3 \cdot pyz = Al(C_6F_5)_3 + pyz$	152.9	147.5	37.9	199.2
$Ga(C_6F_5)_3 \cdot pyz = Ga(C_6F_5)_3 + pyz$	125.2	150.8	31.2	164.2
$In(C_6F_5)_3 \cdot pyz = In(C_6F_5)_3 + pyz$	111.6	130.6	14.7	133.3
$GaI_3 \cdot pyz = GaI_3 + pyz$	115.8	140.1	26.3	151.2
$GaCl_3 \cdot pyz = GaCl_3 + pyz$	135.0	128.6	28.8	86.6
$AlBr_3 \cdot pyz = AlBr_3 + pyz$	152.3	141.2	33.9	97.9
$\{B(C_6F_5)_3\}_2 \cdot pyz = B(C_6F_5)_3 \cdot pyz + B(C_6F_5)_3$	70.9	189.8	110.0	208.2
$\{Al(C_6F_5)_3\}_2 \cdot pyz = Al(C_6F_5)_3 \cdot pyz + Al(C_6F_5)_3$	117.2	163.7	30.4	173.3
$\{Ga(C_6F_5)_3\}_2 \cdot pyz = Ga(C_6F_5)_3 \cdot pyz + Ga(C_6F_5)_3$	95.3	150.9	24.5	142.2
$\{In(C_6F_5)_3\}_2 \cdot pyz = In(C_6F_5)_3 \cdot pyz + In(C_6F_5)_3$	85.4	155.7	10.5	116.1
$(GaI_3)_2 \cdot pyz = GaI_3 \cdot pyz + GaI_3$	87.2	136.2	19.9	115.4
$(GaCl_3)_2 \cdot pyz = GaCl_3 \cdot pyz + GaCl_3$	103.3	142.9	21.5	134.1
$(AlBr_3)_2 \cdot pyz = AlBr_3 \cdot pyz + AlBr_3$	118.3	149.8	26.3	153.8
$pyz \cdot B(C_6F_5)_3 \cdot pyz = B(C_6F_5)_3 \cdot pyz + pyz$	-8.7	136.9	28.8	25.6
$pyz \cdot Al(C_6F_5)_3 \cdot pyz = Al(C_6F_5)_3 \cdot pyz + pyz$	51.7	181.9	55.7	115.1
$pyz \cdot Ga(C_6F_5)_3 \cdot pyz = Ga(C_6F_5)_3 \cdot pyz + pyz$	43.6	164.3	38.0	88.2
$pyz \cdot In(C_6F_5)_3 \cdot pyz = In(C_6F_5)_3 \cdot pyz + pyz$	65.4	165.5	17.4	89.4
$pyz \cdot GaI_3 \cdot pyz = GaI_3 \cdot pyz + pyz$	39.9	152.4	39.8	86.6
$pyz \cdot GaCl_3 \cdot pyz = GaCl_3 \cdot pyz + pyz$	60.7	162.6	40.3	108.7
$pyz \cdot AlBr_3 \cdot pyz = AlBr_3 \cdot pyz + pyz$	61.2	163.6	54.9	124.1

Table S3 Thermodynamic characteristics for the gas phase dissociation processes of studied complexes with hexamethylenetetramine. Standard reaction enthalpies $\Delta_{diss}H°_{298}$ and standard Gibbs energies $\Delta_{diss}G°_{298}$ in kJ mol^{-1}, standard reaction entropies $\Delta_{diss}S°_{298}$ in J mol^{-1} K^{-1}. M06-2X/def2-TZVP level of theory.

Reaction	$\Delta_{diss}H°_{298}$	$\Delta_{diss}S°_{298}$	$\Delta_{diss}G°_{298}$
$(AlMe_3)_4 \cdot hmta = (AlMe_3)_3 \cdot hmta + AlMe_3$	87.0	218.1	22.0
$(AlMe_3)_3 \cdot hmta = (AlMe_3)_2 \cdot hmta + AlMe_3$	96.7	210.1	34.0
$(AlMe_3)_2 \cdot hmta = AlMe_3 \cdot hmta + AlMe_3$	108.0	219.9	42.4
$AlMe_3 \cdot hmta = hmta + AlMe_3$	125.0	190.2	68.3
$(GaMe_3)_4 \cdot hmta = (GaMe_3)_3 \cdot hmta + GaMe_3$	50.9	96.6	22.1
$(GaMe_3)_3 \cdot hmta = (GaMe_3)_2 \cdot hmta + GaMe_3$	78.5	200.1	18.9
$(GaMe_3)_2 \cdot hmta = GaMe_3 \cdot hmta + GaMe_3$	86.9	208.1	24.9
$GaMe_3 \cdot hmta = hmta + GaMe_3$	99.5	182.5	45.1
$(AlCl_3)_4 \cdot hmta = (AlCl_3)_3 \cdot hmta + AlCl_3$	109.3	183.8	54.5
$(AlCl_3)_3 \cdot hmta = (AlCl_3)_2 \cdot hmta + AlCl_3$	130.6	172.3	79.2
$(AlCl_3)_2 \cdot hmta = AlCl_3 \cdot hmta + AlCl_3$	158.6	164.9	109.4
$AlCl_3 \cdot hmta = hmta + AlCl_3$	194.8	155.6	148.4
$(GaCl_3)_4 \cdot hmta = (GaCl_3)_3 \cdot hmta + GaCl_3$	93.6	181.3	39.6
$(GaCl_3)_3 \cdot hmta = (GaCl_3)_2 \cdot hmta + GaCl_3$	113.3	166.5	63.6
$(GaCl_3)_2 \cdot hmta = GaCl_3 \cdot hmta + GaCl_3$	139.1	158.3	91.9
$GaCl_3 \cdot hmta = hmta + GaCl_3$	174.2	153.0	128.6

Table S4 Structural and energetic characteristics of the complexes. R_{DA} – donor acceptor bond distance in Å, $q_{CT}(LA)$ – charge transfer per one LA; WBI_{DA} - Wiberg bond index of the donor-acceptor bond, $\Delta_{diss}H°_{298}$, kJ mol^{-1} – standard dissociation enthalpy of the compound with loss of one LA. M06-2X/def2-TZVP level of theory.

Compound	R_{DA}, exp.	R_{DA}, comput.	$q_{CT(LA)}$	WBI_{DA}	$\Delta_{diss}H°_{298}$
(AlMe₃)·hmta		2.061	0.369	0.195	125.0
(AlMe₃)₂·hmta		2.084	0.331	0.182	108.0
(AlMe₃)₃·hmta	2.101(5), 2.110(5), 2.127(5) [S9]	2.106	0.297	0.170	96.7
(AlMe₃)₄·hmta		2.127	0.264	0.160	87.0
(GaMe₃)·hmta	2.139(17) [S10]	2.174	0.254	0.180	99.5
(GaMe₃)₂·hmta	2.138(9) [S10]	2.199	0.220	0.166	86.9
(GaMe₃)₃·hmta	-	2.223	0.190	0.155	78.5
(GaMe₃)₄·hmta	2.307(9), 2.318(8), 2.276(9), 2.26(1) [S9]	2.245	0.162	0.144	50.9
(AlCl₃)·hmta		1.975	0.408	0.223	194.8
(AlCl₃)₂·hmta		2.005	0.351	0.206	158.6
(AlCl₃)₃·hmta		2.035	0.298	0.191	130.6
(AlCl₃)₄·hmta		2.065	0.251	0.177	109.3
(GaCl₃)·hmta		2.049	0.334	0.225	174.2
(GaCl₃)₂·hmta		2.084	0.271	0.204	139.1
(GaCl₃)₃·hmta		2.119	0.216	0.185	113.3
(GaCl₃)₄·hmta		2.153	0.168	0.169	93.6

Table S5 Structural and energetic characteristics of the pyz complexes. R_{DA} – donor acceptor bond distance in Å, q_{CT} – charge transfer; WBI_{DA} - Wiberg bond index, $\Delta_{diss}H°_{298}$, kJ mol^{-1} – standard dissociation enthalpy of the compound into the components.

Compound	R_{DA},exp.	R_{DA}, comp.	$q_{CT(LA)}$	WBI_{DA}	$\Delta_{diss}H°_{298}$
B(C$_6$F$_5$)$_3$·pyz	1.637(3)	1.639	0.473	0.643	106.6
Al(C$_6$F$_5$)$_3$·pyz	2.025(1)	2.018	0.435	0.268	152.9
Ga(C$_6$F$_5$)$_3$·pyz	2.097(2)	2.114	0.363	0.266	125.2
In(C$_6$F$_5$)$_3$·pyz	-	2.339	0.247	0.239	111.6
GaI$_3$·pyz	2.027(6) [S11]	2.098	0.313	0.248	115.8
GaCl$_3$·pyz	2.203(5)^a [S11], 2.2112(15)^a [S12]	2.073	0.325	0.259	135.0
AlBr$_3$·pyz	2.133(2)^a [S11]	1.996	0.409	0.256	152.3
{B(C$_6$F$_5$)$_3$}$_2$·pyz	1.654(3), 1.661(3) mean 1.658 1.645(2), 1.652(2) mean 1.649 [S13]	1.653	0.410	0.622	177.5
{Al(C$_6$F$_5$)$_3$}$_2$·pyz		2.053	0.358	0.246	270.1
{Ga(C$_6$F$_5$)$_3$}$_2$·pyz	2.091(2)-2.122(2) mean 2.106	2.155	0.284	0.241	220.5
{In(C$_6$F$_5$)$_3$}$_2$·pyz	2.298(3)-2.322(3) mean 2.310	2.385	0.194	0.214	197.0
(GaI$_3$)$_2$·pyz	2.092(6)	2.141	0.240	0.224	202.9
(GaCl$_3$)$_2$·pyz	2.044(7) [S11]	2.111	0.262	0.234	251.8
(AlBr$_3$)$_2$·pyz	1.999(6) [S11]	2.029	0.342	0.236	284.7
pyz·B(C$_6$F$_5$)$_3$·pyz		1.702	0.517	0.615	-8.7
pyz·Al(C$_6$F$_5$)$_3$·pyz		2.217	0.530	0.196	51.7
pyz·Ga(C$_6$F$_5$)$_3$·pyz		2.365	-0.319	0.181	43.6
pyz·In(C$_6$F$_5$)$_3$·pyz		2.492	0.333	0.184	65.4
pyz·GaI$_3$·pyz		2.290	0.329	0.193	155.7
pyz·GaCl$_3$·pyz	2.203(5)^a [S11], 2.2112(15)^a [S12]	2.210	0.355	0.203	209.4
pyz·AlBr$_3$·pyz	2.133(2)^a [S11]	2.138	0.572	0.210	228.0

^{a} 1D polymer.

Table S6 Total energies E°_0, standard enthalpies H°_{298} (in Hartree) and standard entropies S°_{298} (in cal mol^{-1} K^{-1}). M06-2X/def2-TZVP level of theory.

Compound	E°_0	H°_{298}	S°_{298}
Pyz	-264.3030234	-264.220414	65.448
Hmta	-454.8111106	-454.603338	73.106
$B(C_6F_5)_3$	-2208.4735350	-2208.286416	186.829
$Al(C_6F_5)_3$	-2426.0646399	-2425.881037	194.905
$Ga(C_6F_5)_3$	-4108.4809336	-4108.297746	198.100
$In(C_6F_5)_3$	-2373.6768608	-2373.494331	203.573
$AlMe_3$	-362.1473586	-362.031620	92.236
$AlCl_3$	-1623.2364217	-1623.225293	74.733
$GaMe_3$	-2044.5666429	-2044.450497	94.072
$GaCl_3$	-3305.6256704	-3305.615112	77.715
$AlBr_3$	-7965.2136460	-7965.203142	83.135
Al_2Me_6	-724.3321046	-724.097672	125.813
Ga_2Me_6	-4089.1517094	-4088.916664	132.706
$B(C_6F_5)_3 \cdot pyz$	-2472.8202450	-2472.547436	207.468
$Al(C_6F_5)_3 \cdot pyz$	-2690.4284850	-2690.159686	225.101
$Ga(C_6F_5)_3 \cdot pyz$	-4372.8340920	-4372.565835	227.508
$In(C_6F_5)_3 \cdot pyz$	-2638.0246080	-2637.757234	237.796
$pyz \cdot B(C_6F_5)_3 \cdot pyz$	-2737.1220310	-2736.764531	240.188
$pyz \cdot Al(C_6F_5)_3 \cdot pyz$	-2954.7539020	-2954.399774	247.081
$pyz \cdot Ga(C_6F_5)_3 \cdot pyz$	-4637.1560790	-4636.802870	253.691
$pyz \cdot In(C_6F_5)_3 \cdot pyz$	-2902.3548470	-2902.002542	263.688
$B(C_6F_5)_3 \cdot pyz \cdot B(C_6F_5)_3$	-4681.3235400	-4680.860871	348.942
$Al(C_6F_5)_3 \cdot pyz \cdot Al(C_6F_5)_3$	-5116.5401540	-5116.085354	380.890
$Ga(C_6F_5)_3 \cdot pyz \cdot Ga(C_6F_5)_3$	-8481.3536110	-8480.899882	389.543
$In(C_6F_5)_3 \cdot pyz \cdot In(C_6F_5)_3$	-5011.7363280	-5011.284096	404.161
GaI_3	-2817.9216070	-2817.911776	91.810
$GaI_3 \cdot pyz$	-3082.2714480	-3082.176281	123.768
$pyz \cdot GaI_3 \cdot pyz$	-3346.5920000	-3346.411904	152.796
$GaI_3 \cdot pyz \cdot GaI_3$	-5900.2284550	-5900.121251	183.014
$AlMe_3 \bullet hmta$	-817.0082160	-816.682555	119.891
$2AlMe_3 \bullet hmta$	-1179.1995512	-1178.755295	159.589
$3AlMe_3 \bullet hmta$	-1541.3860975	-1540.823728	201.621
$4AlMe_3 \bullet hmta$	-1903.5690904	-1902.888492	241.729
$AlCl_3 \bullet hmta$	-2078.1243161	-2077.902817	110.655
$2AlCl_3 \bullet hmta$	-3701.4239004	-3701.188500	145.993
$3AlCl_3 \bullet hmta$	-5324.7126977	-5324.463539	179.560
$4AlCl_3 \bullet hmta$	-6947.9935219	-6947.730476	210.369
$GaMe_3 \bullet hmta$	-2499.4176475	-2499.091744	123.576
$2GaMe_3 \bullet hmta$	-4544.0198701	-4543.575352	167.926
$3GaMe_3 \bullet hmta$	-6588.6186584	-6588.055762	214.171
$4GaMe_3 \bullet hmta$	-8633.2152394	-8632.533489	257.446
$GaCl_3 \bullet hmta$	-3760.5056903	-3760.284813	114.270
$2GaCl_3 \bullet hmta$	-7066.1869199	-7065.952907	154.168
$3GaCl_3 \bullet hmta$	-10371.8581794	-10371.611160	192.098
$4GaCl_3 \bullet hmta$	-13677.5224289	-13677.261940	226.485
$AlBr_3 \cdot pyz$	-8229.5775131	-8229.481564	114.844
$pyz \cdot AlBr_3 \cdot pyz$	-16194.8387347	-16194.729750	162.170
$AlBr_3 \cdot pyz \cdot AlBr_3$	-8493.9065267	-8493.725284	141.197
$GaCl_3 \cdot pyz$	-3569.9827976	-3569.886947	112.435
$pyz \cdot GaCl_3 \cdot pyz$	-6875.6502644	-6875.541385	156.003
$GaCl_3 \cdot pyz \cdot GaCl_3$	-3834.3114615	-3834.130485	139.010

Table S7 XYZ coordinates of optimized structures. M06-2X/def2-TZVP level of theory.

pyz

N	0.000000000000	0.000000000000	1.396390000000
C	0.000000000000	1.127134000000	0.694770000000
C	0.000000000000	1.127134000000	-0.694770000000
N	0.000000000000	0.000000000000	-1.396390000000
C	0.000000000000	-1.127134000000	-0.694770000000
C	0.000000000000	-1.127134000000	0.694770000000
H	0.000000000000	2.057691000000	1.250713000000
H	0.000000000000	2.057691000000	-1.250713000000
H	0.000000000000	-2.057691000000	-1.250713000000
H	0.000000000000	-2.057691000000	1.250713000000

hmta

N	0.861311000000	-0.861311000000	0.861311000000
N	-0.861311000000	0.861311000000	0.861311000000
N	0.861311000000	0.861311000000	-0.861311000000
C	0.000000000000	1.677645000000	0.000000000000
C	1.677645000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.677645000000
H	0.627829000000	2.313093000000	0.627829000000
H	2.313093000000	0.627829000000	0.627829000000
H	0.627829000000	0.627829000000	2.313093000000
C	0.000000000000	-1.677645000000	0.000000000000
H	-0.627829000000	2.313093000000	-0.627829000000
H	2.313093000000	-0.627829000000	-0.627829000000
H	-0.627829000000	-0.627829000000	2.313093000000
N	-0.861311000000	-0.861311000000	-0.861311000000
C	0.000000000000	0.000000000000	-1.677645000000
H	-0.627829000000	-2.313093000000	0.627829000000
C	-1.677645000000	0.000000000000	0.000000000000
H	0.627829000000	-2.313093000000	-0.627829000000
H	-0.627829000000	0.627829000000	-2.313093000000
H	0.627829000000	-0.627829000000	-2.313093000000
H	-2.313093000000	-0.627829000000	0.627829000000
H	-2.313093000000	0.627829000000	-0.627829000000

B(C$_6$F$_5$)$_3$

B	0.000000000000	0.000000000000	-0.003141000000
C	0.000476000000	1.565144000000	-0.002569000000
C	-0.963091000000	2.308170000000	-0.682579000000
C	0.963810000000	2.306426000000	0.679556000000
C	-0.972754000000	3.689451000000	-0.700678000000
F	-1.919101000000	1.694396000000	-1.376431000000
C	0.973110000000	3.687661000000	0.701773000000
F	1.919750000000	1.691021000000	1.372124000000
C	0.000000000000	4.381428000000	0.001615000000
F	-1.898097000000	4.355208000000	-1.374972000000
F	1.898114000000	4.351747000000	1.378170000000
F	-0.000290000000	5.700374000000	0.003612000000
C	1.355216000000	-0.782984000000	-0.002569000000
C	1.515519000000	-1.987897000000	0.679556000000
C	2.480479000000	-0.320024000000	-0.682579000000
C	2.707053000000	-2.686569000000	0.701773000000

F	0.504592000000	-2.508062000000	1.372124000000
C	3.681535000000	-1.002296000000	-0.700678000000
F	2.426940000000	0.814792000000	-1.376431000000
C	3.794428000000	-2.190714000000	0.001615000000
F	2.819667000000	-3.819688000000	1.378170000000
F	4.720769000000	-0.533804000000	-1.374972000000
F	4.936814000000	-2.849936000000	0.003612000000
C	-1.355693000000	-0.782159000000	-0.002569000000
C	-2.479329000000	-0.318529000000	0.679556000000
C	-1.517388000000	-1.988146000000	-0.682579000000
C	-3.680163000000	-1.001092000000	0.701773000000
F	-2.424342000000	0.817042000000	1.372124000000
C	-2.708782000000	-2.687155000000	-0.700678000000
F	-0.507839000000	-2.509188000000	-1.376431000000
C	-3.794428000000	-2.190714000000	0.001615000000
F	-4.717781000000	-0.532059000000	1.378170000000
F	-2.822672000000	-3.821404000000	-1.374972000000
F	-4.936524000000	-2.850439000000	0.003612000000

Al(C$_6$F$_5$)$_3$

Al	0.000000000000	0.000000000000	0.006687000000
C	-0.000273000000	1.945009000000	0.004477000000
C	1.000735000000	2.678041000000	0.621448000000
C	-1.001032000000	2.674879000000	-0.616484000000
C	1.022043000000	4.060203000000	0.632075000000
F	1.990327000000	2.040287000000	1.255455000000
C	-1.022211000000	4.056982000000	-0.634731000000
F	-1.990385000000	2.033725000000	-1.247520000000
C	0.000000000000	4.748499000000	-0.003260000000
F	1.990671000000	4.731053000000	1.238264000000
F	-1.990596000000	4.724683000000	-1.244761000000
F	0.000240000000	6.069044000000	-0.007009000000
C	-1.684291000000	-0.972741000000	0.004477000000
C	-1.815997000000	-2.204359000000	-0.616484000000
C	-2.819619000000	-0.472359000000	0.621448000000
C	-3.002344000000	-2.913752000000	-0.634731000000
F	-0.766065000000	-2.740586000000	-1.247520000000
C	-4.027261000000	-1.144987000000	0.632075000000
F	-2.762104000000	0.703530000000	1.255455000000
C	-4.112321000000	-2.374250000000	-0.003260000000
F	-3.096397000000	-4.086248000000	-1.244761000000
F	-5.092548000000	-0.641555000000	1.238264000000
F	-5.256066000000	-3.034314000000	-0.007009000000
C	1.684563000000	-0.972268000000	0.004477000000
C	2.817029000000	-0.470520000000	-0.616484000000
C	1.818884000000	-2.205682000000	0.621448000000
C	4.024555000000	-1.143230000000	-0.634731000000
F	2.756450000000	0.706861000000	-1.247520000000
C	3.005218000000	-2.915217000000	0.632075000000
F	0.771777000000	-2.743817000000	1.255455000000
C	4.112321000000	-2.374250000000	-0.003260000000
F	5.086993000000	-0.638435000000	-1.244761000000
F	3.101877000000	-4.089499000000	1.238264000000
F	5.255826000000	-3.034730000000	-0.007009000000

Ga(C₆F₅)₃

Ga	0.000000000000	0.000000000000	0.004880000000
C	-0.000288000000	1.975827000000	0.003290000000
C	1.007818000000	2.703181000000	0.612440000000
C	-1.008136000000	2.700738000000	-0.609111000000
C	1.027631000000	4.085725000000	0.622855000000
F	2.001188000000	2.064079000000	1.236752000000
C	-1.027764000000	4.083251000000	-0.625666000000
F	-2.001361000000	2.059066000000	-1.231092000000
C	0.000000000000	4.774295000000	-0.002946000000
F	2.001644000000	4.756182000000	1.220681000000
F	-2.001553000000	4.751261000000	-1.226568000000
F	0.000238000000	6.095095000000	-0.005951000000
C	-1.710972000000	-0.988163000000	0.003290000000
C	-1.834840000000	-2.223441000000	-0.609111000000
C	-2.844932000000	-0.478795000000	0.612440000000
C	-3.022317000000	-2.931695000000	-0.625666000000
F	-0.782523000000	-2.762762000000	-1.231092000000
C	-4.052157000000	-1.152908000000	0.622855000000
F	-2.788139000000	0.701040000000	1.236752000000
C	-4.134660000000	-2.387147000000	-0.002946000000
F	-3.113936000000	-4.109026000000	-1.226568000000
F	-5.119796000000	-0.644617000000	1.220681000000
F	-5.278627000000	-3.047341000000	-0.005951000000
C	1.711261000000	-0.987664000000	0.003290000000
C	2.842976000000	-0.477298000000	-0.609111000000
C	1.837114000000	-2.224386000000	0.612440000000
C	4.050081000000	-1.151556000000	-0.625666000000
F	2.783884000000	0.703696000000	-1.231092000000
C	3.024526000000	-2.932817000000	0.622855000000
F	0.786951000000	-2.765119000000	1.236752000000
C	4.134660000000	-2.387147000000	-0.002946000000
F	5.115489000000	-0.642235000000	-1.226568000000
F	3.118152000000	-4.111565000000	1.220681000000
F	5.278388000000	-3.047754000000	-0.005951000000

In(C₆F₅)₃

In	0.000000000000	0.000000000000	-0.003646000000
C	0.000000000000	2.157607000000	-0.002151000000
C	1.011393000000	2.880638000000	-0.604399000000
C	-1.011620000000	2.878239000000	0.602517000000
C	1.031936000000	4.263669000000	-0.615445000000
C	-1.032998000000	4.261236000000	0.618037000000
C	-0.000747000000	4.952181000000	0.002378000000
C	-1.868543000000	-1.078804000000	-0.002151000000
C	-3.000402000000	-0.564427000000	-0.604399000000
C	-1.986818000000	-2.315208000000	0.602517000000
C	-4.208414000000	-1.238152000000	-0.615445000000
C	-3.173840000000	-3.025221000000	0.618037000000
C	-4.288341000000	-2.476737000000	0.002378000000
C	1.868543000000	-1.078804000000	-0.002151000000
C	1.989009000000	-2.316211000000	-0.604399000000
C	3.176478000000	-3.025518000000	-0.615445000000

C	4.289088000000	-2.475444000000	0.002378000000
C	4.206838000000	-1.236015000000	0.618037000000
C	2.998438000000	-0.563031000000	0.602517000000
F	-5.279085000000	-0.725964000000	-1.205151000000
F	-5.432663000000	-3.137730000000	0.004549000000
F	-2.942225000000	0.623147000000	-1.218197000000
F	-3.263379000000	-4.207585000000	1.209988000000
F	-0.927395000000	-2.856721000000	1.214805000000
F	-2.010296000000	2.231509000000	1.214805000000
F	-2.012186000000	4.929962000000	1.209988000000
F	-0.001022000000	6.273689000000	0.004549000000
F	2.010839000000	4.934804000000	-1.205151000000
F	2.010773000000	2.236468000000	-1.218197000000
F	0.931452000000	-2.859615000000	-1.218197000000
F	3.268246000000	-4.208839000000	-1.205151000000
F	5.433685000000	-3.135959000000	0.004549000000
F	5.275565000000	-0.722377000000	1.209988000000
F	2.937691000000	0.625213000000	1.214805000000

AlMe₃

C	1.513484000000	-1.237311000000	-0.000021000000
Al	-0.000055000000	-0.000077000000	0.000197000000
C	-1.828419000000	-0.691827000000	0.000291000000
C	0.315031000000	1.929271000000	-0.000389000000
H	1.478668000000	-1.892821000000	-0.875159000000
H	1.476381000000	-1.896211000000	0.872421000000
H	2.482505000000	-0.736526000000	0.001990000000
H	-1.879406000000	-1.781230000000	0.021077000000
H	-2.371279000000	-0.349957000000	-0.885893000000
H	-2.387592000000	-0.314430000000	0.861268000000
H	0.885134000000	2.228386000000	0.884145000000
H	-0.603044000000	2.518087000000	-0.018389000000
H	0.918774000000	2.224911000000	-0.863311000000

AlCl₃

Al	0.000000000000	0.000000000000	0.000000000000
Cl	0.000000000000	2.064826000000	0.000000000000
Cl	-1.788192000000	-1.032413000000	0.000000000000
Cl	1.788192000000	-1.032413000000	0.000000000000

GaMe₃

C	-0.943046000000	1.757287000000	-0.000040000000
Ga	0.000160000000	-0.000004000000	0.000005000000
C	-1.050942000000	-1.694980000000	0.000041000000
C	1.993600000000	-0.062266000000	-0.000006000000
H	-1.589105000000	1.839856000000	0.876906000000
H	-1.592787000000	1.838144000000	-0.874399000000
H	-0.259093000000	2.605030000000	-0.002213000000
H	-2.126899000000	-1.525245000000	0.002722000000
H	-0.796490000000	-2.298702000000	0.874081000000
H	-0.800613000000	-2.295812000000	-0.877205000000
H	2.388614000000	0.457653000000	-0.875702000000
H	2.385118000000	-1.078727000000	0.000021000000
H	2.388607000000	0.457690000000	0.875673000000

GaCl₃

Ga	0.000000000000	0.000000000000	0.000000000000
Cl	0.000000000000	2.124617000000	0.000000000000
Cl	-1.839973000000	-1.062309000000	0.000000000000
Cl	1.839973000000	-1.062309000000	0.000000000000

AlBr₃

Al	0.000000000000	0.000000000000	0.000000000000
Br	0.000000000000	2.228567000000	0.000000000000
Br	1.929995000000	-1.114283000000	0.000000000000
Br	-1.929995000000	-1.114283000000	0.000000000000

Al₂Me₆

Al	1.297695000000	0.010844000000	-0.000136000000
Al	-1.297646000000	0.010794000000	0.000086000000
C	-2.045499000000	1.817049000000	-0.000284000000
C	-2.378736000000	-1.614917000000	0.000283000000
C	2.045284000000	1.817208000000	0.000226000000
C	2.378797000000	-1.614859000000	-0.000177000000
H	-2.672317000000	1.993172000000	0.878103000000
H	-2.676793000000	1.990043000000	-0.876124000000
H	-1.272077000000	2.589005000000	-0.003738000000
H	-3.025952000000	-1.670342000000	0.879305000000
H	-1.755476000000	-2.512992000000	-0.001438000000
H	-3.029015000000	-1.668932000000	-0.876550000000
H	1.271758000000	2.589053000000	0.004896000000
H	2.671086000000	1.993829000000	-0.878786000000
H	2.677529000000	1.989894000000	0.875440000000
H	3.027650000000	-1.669623000000	0.877673000000
H	3.027427000000	-1.669682000000	-0.878184000000
H	1.755474000000	-2.512896000000	-0.000082000000
C	0.000118000000	-0.218641000000	1.676564000000
H	-0.849163000000	0.252178000000	2.188046000000
H	0.003485000000	-1.271621000000	1.961325000000
H	0.846916000000	0.257881000000	2.186911000000
C	-0.000045000000	-0.218815000000	-1.676594000000
H	-0.845985000000	0.258933000000	-2.187196000000
H	-0.004826000000	-1.271862000000	-1.961080000000
H	0.850118000000	0.250522000000	-2.187987000000

Ga₂Me₆

Ga	0.000000000000	1.318374000000	0.013127000000
Ga	0.000000000000	-1.318374000000	0.013127000000
C	0.000000000000	-2.062430000000	1.860377000000
C	0.000000000000	-2.348842000000	-1.687801000000
C	0.000000000000	2.062430000000	1.860377000000
C	0.000000000000	2.348842000000	-1.687801000000
H	0.879604000000	-2.685119000000	2.032183000000
H	-0.879604000000	-2.685119000000	2.032183000000
H	0.000000000000	-1.271172000000	2.611112000000
H	0.880561000000	-2.988531000000	-1.763344000000
H	0.000000000000	-1.674135000000	-2.545506000000
H	-0.880561000000	-2.988531000000	-1.763344000000

H	0.000000000000	1.271172000000	2.611112000000
H	-0.879604000000	2.685119000000	2.032183000000
H	0.879604000000	2.685119000000	2.032183000000
H	0.880561000000	2.988531000000	-1.763344000000
H	-0.880561000000	2.988531000000	-1.763344000000
H	0.000000000000	1.674135000000	-2.545506000000
C	1.768779000000	0.000000000000	-0.215580000000
H	2.268624000000	-0.851768000000	0.259025000000
H	2.041237000000	0.000000000000	-1.270247000000
H	2.268624000000	0.851768000000	0.259025000000
C	-1.768779000000	0.000000000000	-0.215580000000
H	-2.268624000000	-0.851768000000	0.259025000000
H	-2.041237000000	0.000000000000	-1.270247000000
H	-2.268624000000	0.851768000000	0.259025000000

B(C$_6$F$_5$)$_3$·pyz

F	-1.334642000000	-2.514368000000	-0.885229000000
F	2.268477000000	1.072921000000	1.546602000000
F	0.340343000000	-0.751761000000	-2.247851000000
F	-0.992369000000	1.895863000000	-1.764232000000
F	-2.224696000000	1.830153000000	0.730457000000
F	1.893993000000	-1.686124000000	2.109669000000
F	2.181761000000	-2.411468000000	-3.243179000000
F	3.878118000000	-3.721261000000	-1.577570000000
F	-3.862809000000	-2.750479000000	-1.605457000000
F	3.696174000000	-3.326158000000	1.101750000000
F	3.585222000000	3.259969000000	0.769906000000
F	-4.779010000000	1.555071000000	0.015569000000
F	0.332877000000	4.047181000000	-2.516424000000
F	-5.624965000000	-0.736331000000	-1.171367000000
F	2.628188000000	4.772213000000	-1.275538000000
N	-0.325331000000	-0.074265000000	2.035620000000
N	-0.926666000000	-0.252095000000	4.725062000000
C	2.863300000000	-2.702149000000	0.277214000000
C	1.145681000000	-1.388339000000	-1.391703000000
C	-1.634156000000	-0.294410000000	-0.101640000000
C	-0.695646000000	-1.238262000000	2.582005000000
H	-0.746263000000	-2.093849000000	1.921606000000
C	1.897863000000	-1.838572000000	0.775342000000
C	0.991226000000	-1.164922000000	-0.027203000000
C	-2.590692000000	0.687238000000	0.128863000000
C	-3.452490000000	-1.616979000000	-1.051245000000
C	-2.125590000000	-1.455907000000	-0.677984000000
C	0.116676000000	2.188344000000	-1.086598000000
C	1.749223000000	1.797968000000	0.542862000000
C	-0.269637000000	1.000362000000	2.817053000000
H	-0.001419000000	1.938724000000	2.356164000000
C	-0.572563000000	0.893936000000	4.168100000000
H	-0.525548000000	1.769780000000	4.802337000000
C	2.092358000000	-2.234582000000	-1.931942000000
C	0.798208000000	3.319909000000	-1.510158000000
C	-3.920465000000	0.572022000000	-0.222645000000
C	2.960922000000	-2.903706000000	-1.084546000000
C	2.456479000000	2.921614000000	0.159524000000

C	-0.988460000000	-1.314525000000	3.928172000000
H	-1.280191000000	-2.258229000000	4.369988000000
C	0.553038000000	1.389488000000	-0.036946000000
C	1.972015000000	3.692407000000	-0.882673000000
C	-4.354901000000	-0.595606000000	-0.827466000000
B	-0.103377000000	-0.036536000000	0.412576000000

Al(C₆F₅)₃·pyz

Al	-0.003088000000	-0.020142000000	0.212806000000
F	0.778932000000	2.805602000000	1.109210000000
F	1.800241000000	1.638718000000	-1.871160000000
F	2.190450000000	-1.979725000000	1.112590000000
F	-2.535138000000	0.838582000000	-1.595669000000
F	4.753950000000	-2.310228000000	0.363476000000
F	4.352397000000	1.303848000000	-2.602953000000
F	-0.261194000000	5.231702000000	0.604249000000
F	-3.561333000000	3.257421000000	-2.086439000000
F	-3.005956000000	-0.519138000000	0.829129000000
F	-2.437489000000	5.463046000000	-0.995988000000
F	0.560904000000	-2.858635000000	-1.173469000000
F	5.837835000000	-0.667454000000	-1.497053000000
F	-3.703793000000	-4.735858000000	-1.052281000000
F	-4.655037000000	-2.548942000000	0.235265000000
F	-1.092426000000	-4.873567000000	-1.744678000000
N	0.203655000000	-0.007072000000	2.220556000000
N	0.521610000000	0.013105000000	4.969387000000
C	2.494791000000	0.651693000000	-1.294687000000
C	-1.151358000000	-1.601233000000	-0.142874000000
C	-0.314049000000	2.884528000000	0.322054000000
C	2.699241000000	-1.154349000000	0.179821000000
C	4.019099000000	-1.347765000000	-0.180174000000
C	-0.854787000000	1.721971000000	-0.193774000000
C	3.813385000000	0.501296000000	-1.694349000000
C	1.892512000000	-0.163408000000	-0.352654000000
C	-1.955902000000	1.895260000000	-1.013815000000
C	4.576327000000	-0.507124000000	-1.131344000000
C	-1.929416000000	4.267911000000	-0.740556000000
C	-0.717421000000	-2.741450000000	-0.798808000000
C	-2.503745000000	3.136198000000	-1.294361000000
C	-0.818149000000	4.147454000000	0.077570000000
C	-2.497421000000	-1.585651000000	0.180357000000
C	-3.374424000000	-2.613928000000	-0.107031000000
C	-2.890087000000	-3.733513000000	-0.763918000000
C	-1.552642000000	-3.801285000000	-1.113768000000
C	1.309125000000	0.488855000000	2.781905000000
H	2.069217000000	0.880537000000	2.120126000000
C	1.456069000000	0.493033000000	4.159740000000
H	2.353888000000	0.894861000000	4.611626000000
C	-0.743126000000	-0.494427000000	3.026323000000
H	-1.635379000000	-0.894467000000	2.567588000000
C	-0.571986000000	-0.476974000000	4.401725000000
H	-1.341745000000	-0.872234000000	5.052235000000

Ga(C₆F₅)₃·pyz

Ga	-0.014942000000	-0.015289000000	0.115115000000
F	2.029764000000	1.507746000000	-1.846001000000
F	1.961043000000	-2.233086000000	1.006096000000
F	4.569976000000	0.955099000000	-2.501770000000
F	1.070359000000	2.730554000000	1.032223000000
F	-3.052227000000	-0.263917000000	0.821579000000
F	-2.501012000000	1.136031000000	-1.585182000000
F	-3.312118000000	3.654614000000	-2.003289000000
F	0.249428000000	5.256732000000	0.599969000000
F	4.509990000000	-2.783106000000	0.334629000000
F	-1.946580000000	5.722201000000	-0.918263000000
F	-4.156803000000	-4.416517000000	-1.011409000000
F	0.240405000000	-2.886300000000	-1.292272000000
F	-4.882121000000	-2.156817000000	0.296207000000
F	5.816508000000	-1.188313000000	-1.420814000000
F	-1.591710000000	-4.768006000000	-1.795015000000
N	0.208500000000	-0.044516000000	2.217180000000
C	2.608792000000	0.439423000000	-1.288278000000
N	0.557112000000	-0.103782000000	4.960114000000
C	1.900298000000	-0.349797000000	-0.401991000000
C	-1.332943000000	-1.502333000000	-0.209166000000
C	-1.545696000000	4.479582000000	-0.700896000000
C	-0.700411000000	1.840789000000	-0.236020000000
C	3.921804000000	0.176433000000	-1.645462000000
C	-0.030854000000	2.931032000000	0.283028000000
C	-2.658306000000	-1.369467000000	0.162265000000
C	2.581460000000	-1.432292000000	0.124067000000
C	3.891018000000	-1.736676000000	-0.197556000000
C	-1.010822000000	-2.671944000000	-0.874262000000
C	-1.807884000000	2.126051000000	-1.012188000000
C	-3.623820000000	-2.325878000000	-0.089929000000
C	-0.423506000000	4.239669000000	0.075369000000
C	-2.244122000000	3.418759000000	-1.252304000000
C	4.562270000000	-0.920479000000	-1.094647000000
C	-1.940408000000	-3.660695000000	-1.153650000000
C	-3.254713000000	-3.482836000000	-0.756962000000
C	1.357582000000	0.343086000000	2.770949000000
H	2.141852000000	0.679118000000	2.106024000000
C	1.520496000000	0.309171000000	4.147198000000
H	2.454461000000	0.623637000000	4.595386000000
C	-0.580738000000	-0.487087000000	4.397300000000
H	-1.374248000000	-0.827140000000	5.050693000000
C	-0.767228000000	-0.462966000000	3.023248000000
H	-1.695888000000	-0.775064000000	2.567406000000

In(C₆F₅)₃·pyz

F	1.458704000000	-2.641268000000	0.931099000000
F	1.030759000000	-5.292406000000	0.646556000000
F	-1.101938000000	-6.167518000000	-0.773580000000
F	-2.803189000000	-4.400229000000	-1.910195000000
F	-2.379311000000	-1.754802000000	-1.636764000000
F	-3.176568000000	-0.062958000000	0.776390000000
F	-5.257192000000	1.606316000000	0.400610000000

F	-4.884635000000	3.962536000000	-0.880063000000
F	-2.431412000000	4.647862000000	-1.787425000000
F	-0.349250000000	2.983961000000	-1.427718000000
F	1.682092000000	2.531539000000	0.947560000000
F	4.174494000000	3.448429000000	0.465982000000
F	5.811812000000	2.085127000000	-1.202622000000
F	4.962973000000	-0.190481000000	-2.390886000000
F	2.475311000000	-1.107303000000	-1.921499000000
C	-0.450645000000	-2.117867000000	-0.338476000000
C	0.392544000000	-3.055067000000	0.219170000000
C	0.199998000000	-4.418247000000	0.091389000000
C	-0.891669000000	-4.867916000000	-0.634446000000
C	-1.762831000000	-3.959832000000	-1.214414000000
C	-1.524192000000	-2.604963000000	-1.054893000000
C	-1.694131000000	1.405122000000	-0.315088000000
C	-2.964456000000	1.096891000000	0.126323000000
C	-4.051620000000	1.934195000000	-0.047166000000
C	-3.862486000000	3.141572000000	-0.700385000000
C	-2.603859000000	3.490960000000	-1.162142000000
C	-1.548442000000	2.617238000000	-0.960338000000
C	1.997493000000	0.688412000000	-0.478479000000
C	2.473355000000	1.844548000000	0.106452000000
C	3.747093000000	2.335608000000	-0.117643000000
C	4.587927000000	1.637783000000	-0.970530000000
C	4.150712000000	0.471536000000	-1.577282000000
C	2.866622000000	0.021531000000	-1.317718000000
In	-0.035860000000	0.005305000000	-0.058537000000
N	0.181230000000	0.062812000000	2.269723000000
C	-0.846664000000	0.335493000000	3.071708000000
H	-1.810395000000	0.508899000000	2.611109000000
C	1.371241000000	-0.155100000000	2.826528000000
H	2.198877000000	-0.376374000000	2.164110000000
C	1.524861000000	-0.097879000000	4.203865000000
H	2.492415000000	-0.274839000000	4.656578000000
N	0.508936000000	0.172377000000	5.013088000000
C	-0.671179000000	0.387344000000	4.447002000000
H	-1.506806000000	0.608643000000	5.099179000000

pyz·B(C₆F₅)₃·pyz

9	0.906295000	1.724768000	1.791067000
9	1.039473000	-2.863431000	-1.066816000
9	0.494439000	-2.116241000	1.485273000
9	-2.496653000	0.244117000	-0.515319000
9	-1.114729000	1.504346000	-2.477121000
9	3.209555000	1.239931000	-0.467757000
9	2.393649000	-2.622244000	3.195597000
9	4.750104000	-1.279303000	3.122396000
9	-0.169303000	4.082840000	2.162179000
9	5.119128000	0.653725000	1.240872000
9	-0.735645000	-4.797843000	-1.283122000
9	-2.162077000	3.917400000	-2.081666000
9	-4.208689000	-1.696010000	-0.746178000
9	-1.707110000	5.238144000	0.249874000
9	-3.397872000	-4.255597000	-1.133972000

7	1.270811000	0.172894000	-2.236828000
7	2.420254000	0.527881000	-4.752781000
6	3.984551000	-0.035390000	1.282216000
6	1.611248000	-1.398305000	1.345495000
6	-0.042416000	1.475794000	-0.377134000
6	1.759189000	1.356038000	-2.626848000
1	1.690869000	2.176807000	-1.932969000
6	2.969032000	0.224898000	0.381786000
6	1.749575000	-0.440131000	0.344156000
6	-0.843745000	2.120816000	-1.316443000
6	-0.387366000	3.453442000	1.012234000
6	0.166026000	2.197591000	0.789340000
6	-1.973918000	-0.957863000	-0.759305000
6	-0.256556000	-2.507686000	-1.019417000
6	1.350851000	-0.827324000	-3.118969000
1	0.951296000	-1.785198000	-2.845551000
6	1.928432000	-0.638560000	-4.364511000
1	1.982302000	-1.466127000	-5.060155000
6	2.596969000	-1.688739000	2.275021000
6	-2.916105000	-1.974109000	-0.855595000
6	-1.404381000	3.368015000	-1.141162000
6	3.798146000	-1.008844000	2.243790000
6	-1.156193000	-3.549704000	-1.121304000
6	2.328472000	1.518860000	-3.877552000
1	2.715496000	2.486754000	-4.168798000
6	-0.600579000	-1.166172000	-0.855435000
6	-2.510783000	-3.278784000	-1.042914000
6	-1.175051000	4.043969000	0.046794000
5	0.559457000	-0.009014000	-0.701290000
7	-1.450101000	-0.113457000	2.560871000
6	-2.277295000	-1.129266000	2.343267000
6	-3.656993000	-0.984389000	2.432371000
7	-4.222265000	0.175260000	2.744955000
6	-3.394687000	1.186327000	2.979499000
6	-2.015250000	1.041974000	2.891551000
1	-1.355008000	1.876160000	3.102942000
1	-3.837071000	2.139574000	3.245336000
1	-4.316826000	-1.823584000	2.242609000
1	-1.831357000	-2.083530000	2.086181000

pyz·Al(C₆F₅)₃·pyz

Al	0.000066000000	0.004128000000	0.000091000000
F	0.909259000000	-2.692160000000	1.335625000000
F	-0.912339000000	-2.692154000000	-1.332650000000
F	-2.764700000000	0.527418000000	1.563491000000
F	2.764477000000	0.521929000000	-1.564783000000
F	-5.113250000000	-0.740800000000	1.457190000000
F	-3.258891000000	-3.969151000000	-1.398738000000
F	3.254040000000	-3.972418000000	1.401597000000
F	5.111266000000	-0.749667000000	-1.458784000000
F	2.326320000000	2.184160000000	0.428529000000
F	5.374590000000	-3.005366000000	0.017041000000
F	-2.322527000000	2.187924000000	-0.429697000000
F	-5.378923000000	-2.997641000000	-0.016491000000

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F    0.005277000000    6.198393000000   -0.001280000000
F    2.313994000000    4.832124000000    0.403545000000
F   -2.305751000000    4.835875000000   -0.405623000000
N    0.131203000000   -0.051839000000    2.212531000000
N    0.414396000000   -0.128660000000    4.982991000000
C   -1.938641000000   -2.155750000000   -0.649312000000
C    0.001769000000    2.033110000000   -0.000589000000
C    1.935897000000   -2.157919000000    0.651116000000
C   -2.859056000000   -0.550056000000    0.769684000000
C   -4.082188000000   -1.199072000000    0.757168000000
C    1.749536000000   -0.985073000000   -0.058980000000
C   -3.136882000000   -2.848065000000   -0.697678000000
C   -1.751012000000   -0.982445000000    0.059706000000
C    2.857783000000   -0.554976000000   -0.770045000000
C   -4.220558000000   -2.356472000000    0.009149000000
C    4.217133000000   -2.362573000000   -0.008546000000
C   -1.142296000000    2.791273000000   -0.195984000000
C    4.079968000000   -1.205736000000   -0.757674000000
C    3.133193000000   -2.851880000000    0.699453000000
C    1.147112000000    2.789413000000    0.194547000000
C    1.179202000000    4.173927000000    0.200835000000
C    0.004157000000    4.874783000000   -0.001069000000
C   -1.172066000000    4.175843000000   -0.202736000000
C   -0.569867000000   -0.899648000000    2.963353000000
H   -1.245321000000   -1.573619000000    2.457079000000
C   -0.425620000000   -0.929544000000    4.342880000000
H   -1.008030000000   -1.622904000000    4.936696000000
C    0.989194000000    0.745629000000    2.850985000000
H    1.588611000000    1.417527000000    2.256349000000
C    1.123158000000    0.702567000000    4.230192000000
H    1.823226000000    1.359598000000    4.731067000000
N   -0.131418000000   -0.053337000000   -2.212341000000
C   -0.988485000000    0.744978000000   -2.850959000000
C   -1.123301000000    0.700962000000   -4.230057000000
N   -0.416381000000   -0.132121000000   -4.982543000000
C    0.422765000000   -0.933767000000   -4.342237000000
C    0.567941000000   -0.902839000000   -2.962832000000
H    1.242803000000   -1.577276000000   -2.456403000000
H    1.003682000000   -1.628596000000   -4.935795000000
H   -1.822539000000    1.358754000000   -4.731095000000
H   -1.586481000000    1.418340000000   -2.256528000000


pyz·Ga(C₆F₅)₃·pyz
Ga  -0.000007000000   -0.006859000000    0.000109000000
F    0.856109000000    2.716068000000   -1.370217000000
F    2.837705000000   -0.594418000000    1.328873000000
F    3.206549000000    3.991950000000   -1.517045000000
F   -0.850356000000    2.718117000000    1.370011000000
F   -2.229480000000   -2.163785000000    0.780099000000
F   -2.838906000000   -0.588554000000   -1.328647000000
F   -5.184556000000    0.691507000000   -1.154585000000
F   -3.198076000000    3.999031000000    1.516552000000
F    5.186072000000    0.680613000000    1.154534000000
F   -5.378246000000    2.989854000000    0.263096000000
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F	-0.007181000000	-6.188834000000	-0.000091000000
F	2.224682000000	-2.168952000000	-0.779628000000
F	-2.225350000000	-4.827751000000	0.758161000000
F	5.384614000000	2.978319000000	-0.263515000000
F	2.214222000000	-4.832893000000	-0.758121000000
N	0.089249000000	0.064884000000	2.362554000000
C	1.912995000000	2.167650000000	-0.749674000000
N	0.190574000000	0.169012000000	5.141208000000
C	1.763756000000	0.980606000000	-0.058928000000
C	-0.002272000000	-2.039408000000	0.000179000000
C	-4.220867000000	2.349947000000	0.196565000000
C	-1.761640000000	0.984418000000	0.058911000000
C	3.112008000000	2.855186000000	-0.837821000000
C	-1.908384000000	2.171861000000	0.749501000000
C	-1.109010000000	-2.782407000000	0.371267000000
C	2.899177000000	0.515225000000	0.580361000000
C	4.121753000000	1.162578000000	0.524358000000
C	1.102717000000	-2.784967000000	-0.370964000000
C	-2.898033000000	0.521348000000	-0.580334000000
C	-1.137646000000	-4.166870000000	0.382140000000
C	-3.105929000000	2.861966000000	0.837504000000
C	-4.119230000000	1.171306000000	-0.524455000000
C	4.225876000000	2.340890000000	-0.196846000000
C	1.128076000000	-4.169496000000	-0.382026000000
C	-0.005612000000	-4.865350000000	0.000001000000
C	0.785858000000	1.003526000000	2.998895000000
H	1.307871000000	1.732738000000	2.394260000000
C	0.833523000000	1.048730000000	4.384694000000
H	1.406731000000	1.817080000000	4.888693000000
C	-0.508141000000	-0.759391000000	4.502006000000
H	-1.043649000000	-1.484746000000	5.102158000000
C	-0.563231000000	-0.816957000000	3.116368000000
H	-1.144868000000	-1.575749000000	2.613926000000
N	-0.088894000000	0.064855000000	-2.362458000000
C	-0.783528000000	1.004802000000	-2.999037000000
C	-0.830793000000	1.049995000000	-4.384852000000
N	-0.189354000000	0.168998000000	-5.141159000000
C	0.507442000000	-0.760685000000	-4.501732000000
C	0.562081000000	-0.818279000000	-3.116074000000
H	1.142149000000	-1.578152000000	-2.613454000000
H	1.041726000000	-1.487095000000	-5.101704000000
H	-1.402418000000	1.819404000000	-4.889040000000
H	-1.304233000000	1.735098000000	-2.394583000000

pyz·In(C₆F₅)₃·pyz

In	-0.001005000000	0.018032000000	-0.000112000000
F	1.275316000000	-2.625822000000	1.429569000000
F	-0.635888000000	-2.847748000000	-1.436633000000
F	-3.019573000000	0.108818000000	1.341352000000
F	2.918543000000	0.805741000000	-1.338867000000
F	-5.178506000000	-1.487980000000	1.178104000000
F	-2.797459000000	-4.441893000000	-1.584700000000
F	3.745675000000	-3.679862000000	1.579388000000
F	5.386482000000	-0.252067000000	-1.174875000000

F	1.924715000000	2.579056000000	0.803306000000
F	5.804819000000	-2.494193000000	0.281327000000
F	-2.472742000000	2.048982000000	-0.802759000000
F	-5.071940000000	-3.764140000000	-0.281460000000
F	-0.757240000000	6.319227000000	0.002224000000
F	1.597852000000	5.240517000000	0.792199000000
F	-2.788493000000	4.712081000000	-0.789264000000
N	-0.090382000000	-0.037997000000	2.489402000000
N	-0.195904000000	-0.117348000000	5.261163000000
C	-1.751540000000	-2.475755000000	-0.784985000000
C	-0.261716000000	2.210314000000	0.000694000000
C	2.276472000000	-2.005406000000	0.781253000000
C	-2.938965000000	-1.000271000000	0.590436000000
C	-4.062533000000	-1.807803000000	0.533548000000
C	2.015967000000	-0.857801000000	0.061799000000
C	-2.845785000000	-3.318869000000	-0.877723000000
C	-1.760761000000	-1.300397000000	-0.063300000000
C	3.094173000000	-0.293568000000	-0.589937000000
C	-4.010439000000	-2.974945000000	-0.211407000000
C	4.590253000000	-1.970410000000	0.210603000000
C	-1.443300000000	2.808901000000	-0.387997000000
C	4.373259000000	-0.821217000000	-0.532531000000
C	3.535232000000	-2.574400000000	0.874431000000
C	0.743659000000	3.072333000000	0.389808000000
C	0.605263000000	4.450051000000	0.402321000000
C	-0.598812000000	5.004745000000	0.001700000000
C	-1.636484000000	4.180019000000	-0.399604000000
C	-0.675195000000	-1.046376000000	3.129522000000
H	-1.103232000000	-1.837259000000	2.526407000000
C	-0.725366000000	-1.078845000000	4.515965000000
H	-1.205250000000	-1.902498000000	5.029978000000
C	0.446564000000	0.928946000000	3.229190000000
H	0.931629000000	1.745905000000	2.711596000000
C	0.390110000000	0.882251000000	4.615141000000
H	0.829411000000	1.673164000000	5.210592000000
N	0.103475000000	-0.011379000000	-2.489193000000
C	-0.630396000000	0.814896000000	-3.230210000000
C	-0.559221000000	0.784812000000	-4.615963000000
N	0.235839000000	-0.059238000000	-5.260413000000
C	0.961352000000	-0.881831000000	-4.513956000000
C	0.899139000000	-0.864494000000	-3.127749000000
H	1.487997000000	-1.542940000000	-2.523227000000
H	1.613482000000	-1.578039000000	-5.026737000000
H	-1.159930000000	1.460338000000	-5.212537000000
H	-1.285704000000	1.503748000000	-2.713811000000

B(C₆F₅)₃·pyz·B(C₆F₅)₃

F	-3.816730000000	1.594685000000	2.648039000000
F	-2.518572000000	-2.294894000000	-1.220801000000
F	-5.639764000000	0.368081000000	0.943934000000
F	-4.995301000000	1.691265000000	-1.700260000000
F	-2.253273000000	2.267055000000	-1.752872000000
F	-1.726549000000	-2.212515000000	1.486786000000
F	-6.935422000000	-1.274377000000	2.608452000000

F	-5.640311000000	-3.380557000000	3.724773000000
F	-3.885826000000	4.209789000000	3.009611000000
F	-3.026770000000	-3.814009000000	3.133813000000
F	-3.702704000000	-3.274765000000	-3.406194000000
F	-2.310497000000	4.905846000000	-1.352953000000
F	-6.155853000000	0.697611000000	-3.852085000000
F	-3.138674000000	5.904592000000	1.031989000000
F	-5.537869000000	-1.782265000000	-4.744346000000
N	-1.367784000000	0.034465000000	-0.011167000000
N	1.367752000000	-0.034228000000	0.011042000000
C	-3.667707000000	-2.779661000000	2.606551000000
C	-4.962828000000	-0.647469000000	1.487253000000
C	-3.101957000000	1.802587000000	0.395163000000
C	-0.690533000000	0.188823000000	1.125896000000
H	-1.266502000000	0.341863000000	2.028568000000
C	-3.012687000000	-1.912948000000	1.743489000000
C	-3.618228000000	-0.807689000000	1.167753000000
C	-2.691462000000	2.718711000000	-0.566707000000
C	-3.507221000000	3.731129000000	1.833003000000
C	-3.478783000000	2.362519000000	1.606992000000
C	-4.622652000000	0.471148000000	-2.080690000000
C	-3.411760000000	-1.519978000000	-1.859956000000
C	-0.687953000000	-0.146623000000	-1.141637000000
H	-1.249489000000	-0.240917000000	-2.058043000000
C	0.690507000000	-0.188551000000	-1.126011000000
H	1.266432000000	-0.341594000000	-2.028705000000
C	-5.656033000000	-1.485355000000	2.336704000000
C	-5.254754000000	-0.029825000000	-3.209218000000
C	-2.700422000000	4.087072000000	-0.387438000000
C	-4.997707000000	-2.563650000000	2.907154000000
C	-4.009541000000	-2.055742000000	-2.984587000000
C	0.687899000000	0.146899000000	1.141522000000
H	1.249454000000	0.241203000000	2.057920000000
C	-3.668711000000	-0.245148000000	-1.368138000000
C	-4.945262000000	-1.297365000000	-3.667029000000
C	-3.121982000000	4.598922000000	0.829019000000
B	-3.010460000000	0.210374000000	0.050195000000
B	3.010437000000	-0.210353000000	-0.050281000000
C	3.668647000000	0.245350000000	1.368033000000
C	4.622514000000	-0.470856000000	2.080777000000
C	5.254518000000	0.030256000000	3.209288000000
C	4.944994000000	1.297862000000	3.666904000000
C	4.009341000000	2.056152000000	2.984278000000
C	3.411655000000	1.520246000000	1.859660000000
F	2.518511000000	2.295105000000	1.220364000000
F	3.702457000000	3.275227000000	3.405701000000
F	5.537512000000	1.782886000000	4.744214000000
F	6.155554000000	-0.697098000000	3.852342000000
F	4.995155000000	-1.691034000000	1.700530000000
C	3.618355000000	0.807551000000	-1.167939000000
C	3.013016000000	1.912810000000	-1.743875000000
F	1.726911000000	2.212614000000	-1.487252000000
C	3.668184000000	2.779292000000	-2.607052000000
F	3.027412000000	3.813659000000	-3.134485000000

C	4.998168000000	2.563063000000	-2.907563000000
F	5.640917000000	3.379766000000	-3.725268000000
C	5.656316000000	1.484769000000	-2.336901000000
F	6.935692000000	1.273571000000	-2.608541000000
C	4.962948000000	0.647101000000	-1.487371000000
F	5.639750000000	-0.368444000000	-0.943857000000
C	3.101852000000	-1.802582000000	-0.395004000000
C	3.478757000000	-2.362736000000	-1.606719000000
F	3.816746000000	-1.595109000000	-2.647883000000
C	3.507145000000	-3.731386000000	-1.832474000000
F	3.885785000000	-4.210292000000	-3.008979000000
C	3.121823000000	-4.598987000000	-0.828361000000
F	3.138481000000	-5.904691000000	-1.031126000000
C	2.700224000000	-4.086915000000	0.387987000000
F	2.310236000000	-4.905508000000	1.353627000000
C	2.691284000000	-2.718520000000	0.567006000000
F	2.253069000000	-2.266637000000	1.753062000000

Al(C₆F₅)₃·pyz·Al(C₆F₅)₃

Al	-3.425373000000	-0.104237000000	-0.051287000000
F	-3.190149000000	2.585794000000	1.499416000000
F	-2.301874000000	0.249407000000	-2.878455000000
F	-5.489265000000	2.358677000000	-0.131128000000
F	-2.201135000000	-2.693273000000	1.074545000000
F	-4.725717000000	-1.792065000000	2.324497000000
F	-5.197543000000	-1.472254000000	-2.340122000000
F	-5.560495000000	-4.056908000000	-2.940430000000
F	-4.013539000000	3.321964000000	3.943007000000
F	-6.006021000000	4.112063000000	-2.086679000000
F	-2.834267000000	2.014215000000	-4.837261000000
F	-5.526634000000	-1.043767000000	4.758149000000
F	-5.183413000000	1.509128000000	5.582754000000
F	-4.262585000000	-5.972462000000	-1.541612000000
F	-4.689180000000	3.951398000000	-4.442417000000
F	-2.580505000000	-5.290025000000	0.468370000000
C	-3.853281000000	1.253347000000	-1.420057000000
C	-3.689416000000	-1.985282000000	-0.603400000000
N	-1.373688000000	-0.036465000000	-0.014942000000
C	-4.953933000000	-0.160998000000	3.952631000000
C	-4.186030000000	2.071766000000	3.536414000000
C	-3.778164000000	1.658415000000	2.282897000000
C	-3.473677000000	2.097311000000	-3.677984000000
C	-3.921830000000	0.365928000000	1.807579000000
C	-4.533090000000	-2.385434000000	-1.624949000000
C	-4.741495000000	-3.714872000000	-1.956145000000
C	-3.221761000000	1.211507000000	-2.648569000000
C	-4.798153000000	2.253726000000	-1.271398000000
C	-3.051552000000	-3.007242000000	0.078415000000
C	-4.782712000000	1.145625000000	4.377284000000
C	-0.661122000000	-0.848461000000	-0.794997000000
H	-1.202098000000	-1.530196000000	-1.436217000000
C	-3.219853000000	-4.347505000000	-0.210722000000
C	-4.523326000000	-0.521169000000	2.686104000000
C	-0.722048000000	0.811457000000	0.780736000000

H	-1.306404000000	1.469979000000	1.406262000000
C	-5.092582000000	3.168767000000	-2.268385000000
C	-4.421915000000	3.087794000000	-3.477821000000
C	-4.079495000000	-4.698620000000	-1.240837000000
N	1.373728000000	0.036435000000	0.015051000000
C	0.661156000000	0.848428000000	0.795114000000
H	1.202137000000	1.530153000000	1.436337000000
C	0.722086000000	-0.811489000000	-0.780619000000
H	1.306431000000	-1.470019000000	-1.406146000000
Al	3.425433000000	0.104240000000	0.051370000000
F	3.190053000000	-2.585791000000	-1.499357000000
F	2.302154000000	-0.249340000000	2.878527000000
F	5.489268000000	-2.358300000000	0.131045000000
F	2.201413000000	2.693104000000	-1.074924000000
F	4.725982000000	1.791956000000	-2.324380000000
F	5.197076000000	1.472493000000	2.340538000000
F	5.559876000000	4.057221000000	2.940642000000
F	4.013277000000	-3.321963000000	-3.942991000000
F	6.006080000000	-4.112179000000	2.086614000000
F	2.834602000000	-2.014127000000	4.837357000000
F	5.526750000000	1.043648000000	-4.758079000000
F	5.183271000000	-1.509192000000	-5.582738000000
F	4.262264000000	5.972606000000	1.541312000000
F	4.689399000000	-3.951399000000	4.442432000000
F	2.580636000000	5.289932000000	-0.468959000000
C	3.853441000000	-1.253377000000	1.420067000000
C	3.689343000000	1.985318000000	0.603422000000
C	4.953980000000	0.160915000000	-3.952570000000
C	4.185893000000	-2.071787000000	-3.536380000000
C	3.778106000000	-1.658427000000	-2.282840000000
C	3.473936000000	-2.097269000000	3.678041000000
C	3.921886000000	-0.365964000000	-1.807499000000
C	4.532785000000	2.385590000000	1.625113000000
C	4.741099000000	3.715069000000	1.956212000000
C	3.221993000000	-1.211485000000	2.648618000000
C	4.798263000000	-2.253791000000	1.271371000000
C	3.051616000000	3.007196000000	-0.078651000000
C	4.782630000000	-1.145683000000	-4.377250000000
C	3.219843000000	4.347490000000	0.210374000000
C	4.523443000000	0.521095000000	-2.686022000000
C	5.092707000000	-3.168827000000	2.268362000000
C	4.422122000000	-3.087796000000	3.477838000000
C	4.079254000000	4.698728000000	1.240643000000

Ga(C$_6$F$_5$)$_3$·pyz·Ga(C$_6$F$_5$)$_3$

Ga	-3.524614000000	-0.129933000000	-0.006843000000
F	-3.229875000000	2.852162000000	0.899178000000
F	-2.420431000000	-0.451816000000	-2.874515000000
F	-5.545233000000	2.278625000000	-0.657264000000
F	-2.251749000000	-2.369466000000	1.727992000000
F	-4.776100000000	-1.202864000000	2.729107000000
F	-5.165471000000	-2.070446000000	-1.951405000000
F	-5.413558000000	-4.742045000000	-1.967231000000

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F    -3.954397000000      4.130392000000      3.146835000000
F    -6.059534000000      3.552574000000     -2.961044000000
F    -2.949755000000      0.829358000000     -5.183557000000
F    -5.477564000000      0.083353000000      4.967647000000
F    -5.077970000000      2.748852000000      5.188507000000
F    -4.097602000000     -6.237592000000     -0.138540000000
F    -4.770755000000      2.835384000000     -5.227250000000
F    -2.515850000000     -5.050995000000      1.710786000000
C    -3.945878000000      0.884904000000     -1.681746000000
C    -3.708589000000     -2.126197000000     -0.102193000000
N    -1.372075000000     -0.035764000000     -0.001542000000
C    -4.926798000000      0.753490000000      3.965967000000
C    -4.153790000000      2.824369000000      3.034894000000
C    -3.796507000000      2.137185000000      1.890144000000
C    -3.575832000000      1.183196000000     -4.069040000000
C    -3.972582000000      0.775072000000      1.728297000000
C    -4.498529000000     -2.775435000000     -1.032714000000
C    -4.644976000000     -4.153144000000     -1.062309000000
C    -3.324067000000      0.548743000000     -2.867726000000
C    -4.872791000000      1.907929000000     -1.751702000000
C    -3.054982000000     -2.934378000000      0.810002000000
C    -4.726635000000      2.118909000000      4.081170000000
C    -0.666062000000     -0.999057000000     -0.588237000000
H    -1.212128000000     -1.802950000000     -1.062901000000
C    -3.165245000000     -4.312127000000      0.821708000000
C    -4.548533000000      0.111804000000      2.797840000000
C    -0.718245000000      0.962849000000      0.587578000000
H    -1.300726000000      1.742169000000      1.057521000000
C    -5.163462000000      2.576308000000     -2.929500000000
C    -4.506857000000      2.209452000000     -4.092818000000
C    -3.973252000000     -4.921638000000     -0.126244000000
N     1.372084000000      0.035574000000      0.001594000000
C     0.666070000000      0.998872000000      0.588283000000
H     1.212134000000      1.802774000000      1.062931000000
C     0.718253000000     -0.963036000000     -0.587529000000
H     1.300728000000     -1.742356000000     -1.057475000000
Ga    3.524632000000      0.129852000000      0.006842000000
F     3.229849000000     -2.852348000000     -0.898798000000
F     2.420877000000      0.452511000000      2.874526000000
F     5.545153000000     -2.278779000000      0.657580000000
F     2.251718000000      2.368903000000     -1.728515000000
F     4.776274000000      1.202393000000     -2.729182000000
F     5.165064000000      2.070918000000      1.951262000000
F     5.412806000000      4.742551000000      1.966638000000
F     3.954423000000     -4.130891000000     -3.146264000000
F     6.059656000000     -3.552158000000      2.961622000000
F     2.950420000000     -0.828085000000      5.183844000000
F     5.477800000000     -0.084136000000     -4.967528000000
F     5.078130000000     -2.749648000000     -5.188063000000
F     4.096866000000      6.237602000000      0.137530000000
F     4.771256000000     -2.834253000000      5.227817000000
F     2.515473000000      5.050472000000     -1.711761000000
C     3.946052000000     -0.884647000000      1.681908000000
C     3.708394000000      2.126150000000      0.101868000000
```

C	4.926964000000	-0.754124000000	-3.965787000000
C	4.153849000000	-2.824860000000	-3.034482000000
C	3.796536000000	-2.137517000000	-1.889838000000
C	3.576314000000	-1.182270000000	4.069335000000
C	3.972643000000	-0.775388000000	-1.728161000000
C	4.498140000000	2.775655000000	1.032365000000
C	4.644405000000	4.153389000000	1.061733000000
C	3.324437000000	-0.548117000000	2.867887000000
C	4.872883000000	-1.907736000000	1.752005000000
C	3.054781000000	2.934084000000	-0.810542000000
C	4.726763000000	-2.119551000000	-4.080824000000
C	3.164866000000	4.311845000000	-0.822481000000
C	4.548667000000	-0.112275000000	-2.797760000000
C	5.163663000000	-2.575823000000	2.929944000000
C	4.507255000000	-2.208600000000	4.093255000000
C	3.972688000000	4.921629000000	0.125454000000

In(C₆F₅)₃·pyz·In(C₆F₅)₃

In	3.755958000000	-0.069104000000	-0.065808000000
F	3.124375000000	-0.701180000000	-3.195937000000
F	2.636944000000	2.808814000000	0.724289000000
F	5.527574000000	1.158625000000	-2.595656000000
F	2.449107000000	-2.108070000000	2.053379000000
F	4.981994000000	-3.070262000000	0.419255000000
F	5.422602000000	1.522773000000	2.305474000000
F	5.628214000000	1.166311000000	4.967669000000
F	3.549461000000	-2.825452000000	-4.797377000000
F	5.841695000000	3.655951000000	-3.559314000000
F	2.961738000000	5.310677000000	-0.242916000000
F	5.390857000000	-5.189893000000	-1.186279000000
F	4.682329000000	-5.069834000000	-3.792426000000
F	4.257465000000	-0.827503000000	6.173453000000
F	4.564311000000	5.728151000000	-2.384948000000
F	2.667846000000	-2.466789000000	4.720964000000
C	4.069931000000	1.910824000000	-0.910456000000
C	3.938692000000	-0.289313000000	2.097143000000
N	1.371217000000	-0.023870000000	-0.045165000000
C	4.839146000000	-4.086102000000	-1.669429000000
C	3.901397000000	-2.875968000000	-3.519771000000
C	3.701121000000	-1.800940000000	-2.673083000000
C	3.586118000000	4.288767000000	-0.813483000000
C	4.043248000000	-1.816721000000	-1.336581000000
C	4.732061000000	0.528751000000	2.875932000000
C	4.856108000000	0.366391000000	4.245938000000
C	3.440944000000	2.997605000000	-0.341456000000
C	4.877210000000	2.165143000000	-1.999959000000
C	3.256147000000	-1.292648000000	2.754996000000
C	4.478759000000	-4.026714000000	-3.006269000000
C	0.734856000000	0.401691000000	1.042219000000
H	1.336903000000	0.726582000000	1.881435000000
C	3.343126000000	-1.496147000000	4.120354000000
C	4.614357000000	-2.982236000000	-0.864123000000
C	0.650039000000	-0.426213000000	-1.088345000000
H	1.179858000000	-0.765328000000	-1.968654000000

```
C    5.058251000000    3.439036000000   -2.512097000000
C    4.405521000000    4.503694000000   -1.910884000000
C    4.155309000000   -0.655574000000    4.866398000000
N   -1.371217000000    0.023870000000    0.045165000000
C   -0.734856000000   -0.401691000000   -1.042219000000
H   -1.336903000000   -0.726582000000   -1.881435000000
C   -0.650039000000    0.426213000000    1.088345000000
H   -1.179858000000    0.765328000000    1.968654000000
In  -3.755958000000    0.069104000000    0.065808000000
F   -3.124375000000    0.701180000000    3.195937000000
F   -2.636944000000   -2.808814000000   -0.724289000000
F   -5.527574000000   -1.158625000000    2.595656000000
F   -2.449107000000    2.108070000000   -2.053379000000
F   -4.981994000000    3.070262000000   -0.419255000000
F   -5.422602000000   -1.522773000000   -2.305474000000
F   -5.628214000000   -1.166311000000   -4.967669000000
F   -3.549461000000    2.825452000000    4.797377000000
F   -5.841695000000   -3.655951000000    3.559314000000
F   -2.961738000000   -5.310677000000    0.242916000000
F   -5.390857000000    5.189893000000    1.186279000000
F   -4.682329000000    5.069834000000    3.792426000000
F   -4.257465000000    0.827503000000   -6.173453000000
F   -4.564311000000   -5.728151000000    2.384948000000
F   -2.667846000000    2.466789000000   -4.720964000000
C   -4.069931000000   -1.910824000000    0.910456000000
C   -3.938692000000    0.289313000000   -2.097143000000
C   -4.839146000000    4.086102000000    1.669429000000
C   -3.901397000000    2.875968000000    3.519771000000
C   -3.701121000000    1.800940000000    2.673083000000
C   -3.586118000000   -4.288767000000    0.813483000000
C   -4.043248000000    1.816721000000    1.336581000000
C   -4.732061000000   -0.528751000000   -2.875932000000
C   -4.856108000000   -0.366391000000   -4.245938000000
C   -3.440944000000   -2.997605000000    0.341456000000
C   -4.877210000000   -2.165143000000    1.999959000000
C   -3.256147000000    1.292648000000   -2.754996000000
C   -4.478759000000    4.026714000000    3.006269000000
C   -3.343126000000    1.496147000000   -4.120354000000
C   -4.614357000000    2.982236000000    0.864123000000
C   -5.058251000000   -3.439036000000    2.512097000000
C   -4.405521000000   -4.503694000000    1.910884000000
C   -4.155309000000    0.655574000000   -4.866398000000
```

GaI₃

```
Ga   0.000000000000    0.000000000000    0.000000000000
I    0.000000000000    2.481256000000    0.000000000000
I    2.148831000000   -1.240628000000    0.000000000000
I   -2.148831000000   -1.240628000000    0.000000000000
```

GaI₃·pyz

```
I   -0.162501000000   -1.822834000000   -1.824996000000
I    0.051621000000   -1.011077000000    2.363201000000
I   -1.971427000000    1.749007000000   -0.252249000000
Ga  -0.263999000000   -0.095906000000    0.024690000000
```

N	1.578718000000	0.871600000000	-0.241283000000
N	4.074408000000	2.013556000000	-0.519645000000
C	1.712723000000	2.191718000000	-0.346093000000
C	2.974920000000	2.752489000000	-0.485919000000
C	3.922763000000	0.698821000000	-0.411239000000
C	2.675953000000	0.112943000000	-0.270470000000
H	0.808907000000	2.786707000000	-0.318647000000
H	3.088730000000	3.825700000000	-0.572423000000
H	4.815503000000	0.087147000000	-0.437182000000
H	2.543035000000	-0.958444000000	-0.183955000000

pyz·GaI$_3$·pyz

I	-0.344981000000	-2.193823000000	-1.356537000000
I	-0.000037000000	-0.002123000000	2.532271000000
I	0.345163000000	2.195933000000	-1.353120000000
Ga	-0.000101000000	0.000042000000	-0.050836000000
N	2.277917000000	-0.222406000000	0.022697000000
N	5.044381000000	-0.279727000000	0.237846000000
C	2.944095000000	0.748097000000	0.648569000000
C	4.324344000000	0.711923000000	0.751271000000
C	4.373012000000	-1.238262000000	-0.381788000000
C	2.987582000000	-1.218738000000	-0.495231000000
H	2.363674000000	1.558509000000	1.070328000000
H	4.856769000000	1.504555000000	1.261729000000
H	4.943080000000	-2.055139000000	-0.806913000000
H	2.446324000000	-2.004783000000	-1.003052000000
N	-2.278005000000	0.222296000000	0.023183000000
C	-2.944473000000	-0.749056000000	0.647420000000
H	-2.364320000000	-1.560275000000	1.068013000000
C	-4.324738000000	-0.712746000000	0.749976000000
H	-4.857392000000	-1.506064000000	1.259124000000
N	-5.044501000000	0.279812000000	0.237947000000
C	-4.372847000000	1.239161000000	-0.380130000000
H	-4.942697000000	2.056793000000	-0.804096000000
C	-2.987410000000	1.219560000000	-0.493353000000
H	-2.445942000000	2.006292000000	-0.999878000000

GaI$_3$·pyz·GaI$_3$

I	-3.843668000000	0.951948000000	2.331681000000
I	-4.128406000000	-2.413421000000	-0.358542000000
I	-3.864287000000	1.614071000000	-1.892548000000
Ga	-3.505243000000	0.000826000000	0.016678000000
N	-1.365088000000	-0.050243000000	-0.001525000000
C	-0.651541000000	-1.158099000000	-0.185445000000
H	-1.193371000000	-2.083367000000	-0.333342000000
C	-0.732138000000	1.105909000000	0.183660000000
H	-1.337657000000	1.991523000000	0.330952000000
I	3.843668000000	-0.951948000000	-2.331681000000
I	4.128406000000	2.413421000000	0.358542000000
I	3.864287000000	-1.614071000000	1.892548000000
Ga	3.505243000000	-0.000826000000	-0.016678000000
N	1.365088000000	0.050243000000	0.001525000000
C	0.651541000000	1.158099000000	0.185445000000
H	1.193371000000	2.083367000000	0.333342000000

| C | 0.732138000000 | -1.105909000000 | -0.183660000000 |
| H | 1.337657000000 | -1.991523000000 | -0.330952000000 |

AlMe₃•hmta

N	1.820516000000	0.277933000000	1.372494000000
N	1.820536000000	1.050168000000	-0.927179000000
N	1.820924000000	-1.328066000000	-0.445745000000
C	2.294696000000	-0.272299000000	-1.344893000000
C	2.294567000000	-1.028573000000	0.908421000000
C	2.294084000000	1.301359000000	0.436588000000
H	3.385415000000	-0.273071000000	-1.347872000000
H	3.385296000000	-1.030878000000	0.910926000000
H	3.384815000000	1.305207000000	0.437453000000
C	0.370318000000	0.281316000000	1.363936000000
H	1.937428000000	-0.476644000000	-2.355499000000
H	1.937172000000	-1.801481000000	1.590802000000
H	1.936214000000	2.278517000000	0.765056000000
N	-0.171505000000	-0.000566000000	-0.000775000000
C	0.370545000000	-1.322818000000	-0.438730000000
H	-0.004424000000	1.255625000000	1.678153000000
C	0.370160000000	1.040398000000	-0.926693000000
H	-0.013388000000	-0.483755000000	2.041093000000
Al	-2.232452000000	0.000029000000	0.000325000000
H	-0.012900000000	-1.527129000000	-1.439936000000
H	-0.004290000000	-2.082226000000	0.247757000000
H	-0.014389000000	2.009361000000	-0.603489000000
H	-0.003874000000	0.824980000000	-1.927752000000
C	-2.624993000000	1.634992000000	1.049217000000
C	-2.626828000000	-1.725372000000	0.891596000000
C	-2.628958000000	0.091265000000	-1.939095000000
H	-3.688120000000	1.880447000000	0.965463000000
H	-2.085475000000	2.524878000000	0.707110000000
H	-2.420785000000	1.522090000000	2.118246000000
H	-3.693335000000	-0.100217000000	-2.106396000000
H	-2.093955000000	-0.652400000000	-2.539701000000
H	-2.422546000000	1.072511000000	-2.377142000000
H	-3.691181000000	-1.776253000000	1.140831000000
H	-2.091807000000	-1.872761000000	1.836067000000
H	-2.418838000000	-2.595067000000	0.260962000000

2AlMe₃•hmta

N	-0.000002000000	-1.992067000000	1.208243000000
N	-0.000002000000	-1.990789000000	-1.209206000000
N	-1.218165000000	-0.274403000000	0.000466000000
C	-1.185843000000	-1.155593000000	-1.204965000000
C	-1.180661000000	-1.149156000000	1.210127000000
C	-0.000003000000	-2.818957000000	-0.000682000000
H	-2.080951000000	-1.776136000000	-1.190574000000
H	-2.082539000000	-1.762182000000	1.207996000000
H	-0.888194000000	-3.451182000000	-0.000975000000
C	1.180656000000	-1.149155000000	1.210130000000
Al	-2.920551000000	0.927776000000	-0.000191000000
H	-1.204838000000	-0.517800000000	-2.089934000000
H	-1.184787000000	-0.507734000000	2.091130000000

H	0.888188000000	-3.451183000000	-0.000974000000
N	1.218164000000	-0.274405000000	0.000466000000
C	0.000000000000	0.560876000000	-0.010809000000
H	2.082536000000	-1.762179000000	1.208001000000
C	1.185843000000	-1.155599000000	-1.204963000000
H	1.184781000000	-0.507732000000	2.091132000000
Al	2.920553000000	0.927774000000	-0.000191000000
H	-0.000001000000	1.177354000000	-0.908637000000
H	0.000001000000	1.207912000000	0.868242000000
H	2.080948000000	-1.776146000000	-1.190570000000
H	1.204843000000	-0.517807000000	-2.089933000000
C	4.305779000000	-0.401856000000	-0.483063000000
C	2.918655000000	1.564032000000	1.873605000000
C	2.430208000000	2.247705000000	-1.389610000000
C	-2.430090000000	2.247868000000	-1.389417000000
C	-2.918805000000	1.563815000000	1.873680000000
C	-4.305739000000	-0.401797000000	-0.483331000000
H	5.298288000000	0.030576000000	-0.324142000000
H	4.269914000000	-0.703417000000	-1.534155000000
H	4.280836000000	-1.315841000000	0.120300000000
H	3.306126000000	2.849749000000	-1.649632000000
H	1.660702000000	2.955189000000	-1.065863000000
H	2.086605000000	1.803008000000	-2.329934000000
H	3.638965000000	2.380300000000	1.983732000000
H	3.216813000000	0.795872000000	2.593434000000
H	1.958172000000	1.970161000000	2.209296000000
H	-4.269790000000	-0.703234000000	-1.534456000000
H	-5.298261000000	0.030618000000	-0.324441000000
H	-4.280848000000	-1.315853000000	0.119925000000
H	-1.660608000000	2.955313000000	-1.065525000000
H	-3.305986000000	2.849945000000	-1.649438000000
H	-2.086412000000	1.803281000000	-2.329765000000
H	-1.958351000000	1.969903000000	2.209500000000
H	-3.217026000000	0.795571000000	2.593395000000
H	-3.639123000000	2.380071000000	1.983843000000

3AlMe₃•hmta

N	-1.161309000000	0.786585000000	-0.288206000000
N	-0.100203000000	-1.398670000000	-0.289652000000
N	-0.000201000000	0.001262000000	-2.260861000000
C	-0.092498000000	-1.364691000000	-1.780871000000
C	-1.130247000000	0.773011000000	-1.779717000000
C	-1.252926000000	-0.608494000000	0.185962000000
H	-1.012946000000	-1.830406000000	-2.133568000000
H	-2.065315000000	0.337862000000	-2.132962000000
H	-2.170262000000	-1.053469000000	-0.194761000000
C	0.099169000000	1.382939000000	0.196760000000
H	0.761579000000	-1.944272000000	-2.128105000000
H	-1.057811000000	1.803169000000	-2.125383000000
H	-1.271990000000	-0.618928000000	1.276946000000
N	1.261788000000	0.613259000000	-0.288897000000
C	1.233694000000	0.594133000000	-1.780049000000
H	0.101487000000	1.384963000000	1.286773000000
C	1.141937000000	-0.772985000000	0.205141000000

H	0.170343000000	2.407663000000	-0.166503000000
H	2.089487000000	0.016692000000	-2.126588000000
H	1.323942000000	1.621701000000	-2.132779000000
H	1.128809000000	-0.764255000000	1.293885000000
H	1.998301000000	-1.353026000000	-0.140999000000
Al	-0.242660000000	-3.378023000000	0.415548000000
C	1.084369000000	-4.253124000000	-0.760619000000
H	2.054884000000	-3.746510000000	-0.801481000000
H	1.294289000000	-5.259493000000	-0.386000000000
H	0.737647000000	-4.379216000000	-1.790565000000
C	-2.151114000000	-3.732598000000	0.040844000000
H	-2.356343000000	-4.799189000000	0.173009000000
H	-2.833919000000	-3.207150000000	0.715387000000
H	-2.460906000000	-3.497782000000	-0.983363000000
C	0.272832000000	-3.099869000000	2.302883000000
H	-0.276355000000	-2.297366000000	2.807540000000
H	0.060153000000	-4.006831000000	2.876774000000
H	1.339657000000	-2.898348000000	2.439332000000
Al	-2.806052000000	1.897434000000	0.415046000000
C	-4.263927000000	0.616836000000	0.037405000000
H	-4.269118000000	0.227380000000	-0.986505000000
H	-4.275287000000	-0.244221000000	0.712502000000
H	-5.229040000000	1.115796000000	0.167114000000
C	-2.672010000000	3.483966000000	-0.757294000000
H	-2.979947000000	3.291450000000	-1.789303000000
H	-3.337031000000	4.268557000000	-0.384008000000
H	-1.674548000000	3.935827000000	-0.791294000000
C	-2.274312000000	2.128993000000	2.304552000000
H	-3.124940000000	2.508654000000	2.878506000000
H	-1.971217000000	1.203444000000	2.806372000000
H	-1.467240000000	2.854533000000	2.443929000000
Al	3.047919000000	1.478700000000	0.415303000000
C	2.671351000000	3.383215000000	0.040601000000
H	2.323504000000	3.583606000000	-0.978694000000
H	1.943561000000	3.826340000000	0.726971000000
H	3.590427000000	3.965374000000	0.157129000000
C	2.983612000000	0.898311000000	2.302662000000
H	3.751623000000	1.428708000000	2.873665000000
H	2.037219000000	1.116568000000	2.809586000000
H	3.187275000000	-0.168070000000	2.439451000000
C	4.351174000000	0.571305000000	-0.763103000000
H	4.338898000000	0.940569000000	-1.792860000000
H	5.363904000000	0.749304000000	-0.389096000000
H	4.240381000000	-0.517810000000	-0.804350000000

4AlMe₃•hmta

Al	-2.232557000000	1.957504000000	2.053792000000
N	-0.916458000000	0.804321000000	0.844963000000
N	0.895300000000	-0.803476000000	0.868101000000
N	-0.793231000000	-0.906382000000	-0.865878000000
C	0.110148000000	-1.695494000000	-0.006249000000
C	-1.695446000000	-0.110120000000	-0.012192000000
C	-0.021040000000	0.000826000000	1.699379000000
H	-0.479864000000	-2.376029000000	0.608623000000

H	-2.276904000000	-0.781173000000	0.616963000000
H	-0.620939000000	-0.662860000000	2.320972000000
C	-0.110099000000	1.695399000000	-0.010852000000
Al	2.180915000000	-1.954784000000	2.110565000000
Al	-1.930327000000	-2.207964000000	-2.104992000000
H	0.789294000000	-2.269640000000	-0.633451000000
H	-2.368697000000	0.471822000000	-0.642544000000
H	0.563249000000	0.665123000000	2.335015000000
N	0.814400000000	0.905531000000	-0.847139000000
C	0.021012000000	-0.000951000000	-1.699353000000
H	0.464354000000	2.376833000000	0.617606000000
C	1.695167000000	0.110084000000	0.029413000000
H	-0.773608000000	2.268480000000	-0.655489000000
Al	1.981938000000	2.205601000000	-2.059350000000
H	0.692782000000	-0.593486000000	-2.319330000000
H	-0.635100000000	0.590755000000	-2.336658000000
H	2.260907000000	0.781791000000	0.672044000000
H	2.383755000000	-0.472612000000	-0.583498000000
C	3.233833000000	2.873497000000	-0.685445000000
C	0.558063000000	3.428903000000	-2.671800000000
C	2.673836000000	0.887505000000	-3.357795000000
C	-0.932066000000	2.633471000000	3.378087000000
C	-3.463653000000	0.526335000000	2.632728000000
C	-2.882301000000	3.225691000000	0.686158000000
C	-0.491674000000	-3.432679000000	-2.679084000000
C	-2.587971000000	-0.892070000000	-3.423349000000
C	-3.217231000000	-2.873204000000	-0.762610000000
C	3.398074000000	-0.523083000000	2.717139000000
C	2.863328000000	-3.226347000000	0.762155000000
C	0.848010000000	-2.628112000000	3.403693000000
H	1.296077000000	-3.424884000000	4.004884000000
H	-0.043025000000	-3.072775000000	2.946787000000
H	0.507085000000	-1.869068000000	4.114086000000
H	3.250299000000	-2.756864000000	-0.148975000000
H	2.127350000000	-3.975451000000	0.454851000000
H	3.704878000000	-3.784632000000	1.183102000000
H	4.089513000000	-0.177870000000	1.942560000000
H	4.022361000000	-0.898998000000	3.533262000000
H	2.891033000000	0.360735000000	3.119819000000
H	3.796922000000	3.720646000000	-1.088358000000
H	3.979463000000	2.134818000000	-0.376198000000
H	2.750928000000	3.249088000000	0.223446000000
H	3.476851000000	1.343530000000	-3.944530000000
H	1.924394000000	0.552305000000	-4.080987000000
H	3.114966000000	-0.007161000000	-2.904645000000
H	0.945499000000	4.063796000000	-3.474250000000
H	0.200496000000	4.110220000000	-1.893855000000
H	-0.319003000000	2.926128000000	-3.094092000000
H	-2.757743000000	-3.250430000000	0.157656000000
H	-3.772014000000	-3.718884000000	-1.179922000000
H	-3.968766000000	-2.133145000000	-0.471538000000
H	0.395708000000	-2.930529000000	-3.080058000000
H	-0.858919000000	-4.068811000000	-3.490004000000
H	-0.153724000000	-4.112817000000	-1.891414000000

```
H   -1.820074000000   -0.560116000000   -4.128458000000
H   -3.038483000000    0.004679000000   -2.983669000000
H   -3.376971000000   -1.348133000000   -4.028744000000
H   -2.966244000000   -0.356910000000    3.048488000000
H   -4.136312000000    0.180035000000    1.842258000000
H   -4.107310000000    0.903076000000    3.433276000000
H   -0.031235000000    3.079806000000    2.942573000000
H   -0.606797000000    1.875149000000    4.096547000000
H   -1.395880000000    3.429408000000    3.968342000000
H   -2.139741000000    3.975093000000    0.395972000000
H   -3.734985000000    3.783791000000    1.084304000000
H   -3.245446000000    2.753660000000   -0.233442000000
```

AlCl$_3$•hmta
```
N    0.000000000000    1.398212000000   -2.254322000000
N   -1.210887000000   -0.699106000000   -2.254322000000
N    1.210887000000   -0.699106000000   -2.254322000000
C    0.000000000000   -1.373859000000   -2.728857000000
C    1.189797000000    0.686930000000   -2.728857000000
C   -1.189797000000    0.686930000000   -2.728857000000
H    0.000000000000   -1.376661000000   -3.819179000000
H    1.192223000000    0.688330000000   -3.819179000000
H   -1.192223000000    0.688330000000   -3.819179000000
C    0.000000000000    1.405911000000   -0.810427000000
H    0.000000000000   -2.404273000000   -2.370529000000
H    2.082162000000    1.202137000000   -2.370529000000
H   -2.082162000000    1.202137000000   -2.370529000000
N    0.000000000000    0.000000000000   -0.257007000000
C    1.217554000000   -0.702955000000   -0.810427000000
H   -0.890240000000    1.908093000000   -0.430201000000
C   -1.217554000000   -0.702955000000   -0.810427000000
H    0.890240000000    1.908093000000   -0.430201000000
Al   0.000000000000    0.000000000000    1.718378000000
H    1.207337000000   -1.725017000000   -0.430201000000
H    2.097577000000   -0.183076000000   -0.430201000000
H   -2.097577000000   -0.183076000000   -0.430201000000
H   -1.207337000000   -1.725017000000   -0.430201000000
Cl   0.000000000000   -2.063449000000    2.189379000000
Cl   1.786999000000    1.031725000000    2.189379000000
Cl  -1.786999000000    1.031725000000    2.189379000000
```

2AlCl$_3$•hmta
```
Al   0.000000000000    2.872679000000   -0.629662000000
N    0.000000000000    1.221923000000    0.508827000000
N    1.203797000000    0.000000000000    2.226650000000
N   -1.203797000000    0.000000000000    2.226650000000
C    0.000000000000    0.000000000000    3.059793000000
C   -1.218936000000    1.182119000000    1.397936000000
C    1.218936000000    1.182119000000    1.397936000000
H    0.000000000000    0.888671000000    3.690393000000
H   -1.205746000000    2.080927000000    2.013404000000
H    1.205746000000    2.080927000000    2.013404000000
C    0.000000000000    0.000000000000   -0.335534000000
H    0.000000000000   -0.888671000000    3.690393000000
```

H	-2.099035000000	1.190962000000	0.754752000000
H	2.099035000000	1.190962000000	0.754752000000
N	0.000000000000	-1.221923000000	0.508827000000
C	-1.218936000000	-1.182119000000	1.397936000000
H	0.891847000000	0.000000000000	-0.963809000000
C	1.218936000000	-1.182119000000	1.397936000000
H	-0.891847000000	0.000000000000	-0.963809000000
Al	0.000000000000	-2.872679000000	-0.629662000000
H	-1.205746000000	-2.080927000000	2.013404000000
H	-2.099035000000	-1.190962000000	0.754752000000
H	2.099035000000	-1.190962000000	0.754752000000
H	1.205746000000	-2.080927000000	2.013404000000
Cl	0.000000000000	4.395836000000	0.834923000000
Cl	1.792286000000	2.643821000000	-1.716686000000
Cl	-1.792286000000	2.643821000000	-1.716686000000
Cl	-1.792286000000	-2.643821000000	-1.716686000000
Cl	0.000000000000	-4.395836000000	0.834923000000
Cl	1.792286000000	-2.643821000000	-1.716686000000

3AlCl₃•hmta

Al	2.885600000000	1.666002000000	-0.260383000000
N	1.217577000000	0.702968000000	0.396911000000
N	0.000000000000	0.000000000000	2.362052000000
N	-1.217577000000	0.702968000000	0.396911000000
C	-1.185354000000	0.684365000000	1.903066000000
C	0.000000000000	1.394971000000	-0.094265000000
C	1.185354000000	0.684365000000	1.903066000000
H	-1.191844000000	1.717453000000	2.247889000000
H	0.000000000000	2.420867000000	0.273767000000
H	1.191844000000	1.717453000000	2.247889000000
C	1.208080000000	-0.697485000000	-0.094265000000
Al	-2.885600000000	1.666002000000	-0.260383000000
H	-2.083280000000	0.173441000000	2.247889000000
H	0.000000000000	1.391729000000	-1.184988000000
H	2.083280000000	0.173441000000	2.247889000000
N	0.000000000000	-1.405937000000	0.396911000000
C	-1.208080000000	-0.697485000000	-0.094265000000
H	2.096532000000	-1.210433000000	0.273767000000
C	0.000000000000	-1.368729000000	1.903066000000
H	1.205273000000	-0.695864000000	-1.184988000000
Al	0.000000000000	-3.332004000000	-0.260383000000
H	-2.096532000000	-1.210433000000	0.273767000000
H	-1.205273000000	-0.695864000000	-1.184988000000
H	0.891436000000	-1.890894000000	2.247889000000
H	-0.891436000000	-1.890894000000	2.247889000000
Cl	2.596063000000	3.566064000000	0.602002000000
Cl	4.386334000000	0.465225000000	0.602002000000
Cl	2.627932000000	1.517237000000	-2.341781000000
Cl	0.000000000000	-3.034474000000	-2.341781000000
Cl	-1.790271000000	-4.031289000000	0.602002000000
Cl	1.790271000000	-4.031289000000	0.602002000000
Cl	-2.627932000000	1.517237000000	-2.341781000000
Cl	-4.386334000000	0.465225000000	0.602002000000
Cl	-2.596063000000	3.566064000000	0.602002000000

4AlCl₃•hmta

Al	2.049840000000	-2.049840000000	2.049840000000
N	0.857752000000	-0.857752000000	0.857752000000
N	-0.857752000000	0.857752000000	0.857752000000
N	0.857752000000	0.857752000000	-0.857752000000
C	0.000000000000	1.710473000000	0.000000000000
C	1.710473000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.710473000000
H	0.631731000000	2.334712000000	0.631731000000
H	2.334712000000	0.631731000000	0.631731000000
H	0.631731000000	0.631731000000	2.334712000000
C	0.000000000000	-1.710473000000	0.000000000000
Al	-2.049840000000	2.049840000000	2.049840000000
Al	2.049840000000	2.049840000000	-2.049840000000
H	-0.631731000000	2.334712000000	-0.631731000000
H	2.334712000000	-0.631731000000	-0.631731000000
H	-0.631731000000	-0.631731000000	2.334712000000
N	-0.857752000000	-0.857752000000	-0.857752000000
C	0.000000000000	0.000000000000	-1.710473000000
H	-0.631731000000	-2.334712000000	0.631731000000
C	-1.710473000000	0.000000000000	0.000000000000
H	0.631731000000	-2.334712000000	-0.631731000000
Al	-2.049840000000	-2.049840000000	-2.049840000000
H	-0.631731000000	0.631731000000	-2.334712000000
H	0.631731000000	-0.631731000000	-2.334712000000
H	-2.334712000000	-0.631731000000	0.631731000000
H	-2.334712000000	0.631731000000	-0.631731000000
Cl	3.098494000000	-0.562079000000	3.098494000000
Cl	0.562079000000	-3.098494000000	3.098494000000
Cl	3.098494000000	-3.098494000000	0.562079000000
Cl	-0.562079000000	-3.098494000000	-3.098494000000
Cl	-3.098494000000	-0.562079000000	-3.098494000000
Cl	-3.098494000000	-3.098494000000	-0.562079000000
Cl	3.098494000000	0.562079000000	-3.098494000000
Cl	0.562079000000	3.098494000000	-3.098494000000
Cl	-0.562079000000	3.098494000000	3.098494000000
Cl	-3.098494000000	0.562079000000	3.098494000000
Cl	-3.098494000000	3.098494000000	0.562079000000
Cl	3.098494000000	3.098494000000	-0.562079000000

GaMe₃•hmta

N	-2.155281000000	-0.185402000000	-1.389712000000
N	-2.155217000000	1.296083000000	0.534500000000
N	-2.154287000000	-1.111054000000	0.855272000000
C	-2.627792000000	0.180973000000	1.360290000000
C	-2.627834000000	-1.268859000000	-0.522984000000
C	-2.628788000000	1.087212000000	-0.836729000000
H	-3.718629000000	0.180903000000	1.364590000000
H	-3.718671000000	-1.272947000000	-0.524349000000
H	-3.719648000000	1.090201000000	-0.838632000000
C	-0.702450000000	-0.178659000000	-1.377896000000
H	-2.269963000000	0.317576000000	2.382154000000
H	-2.270064000000	-2.222035000000	-0.915905000000

```
H   -2.271699000000     1.904144000000    -1.466018000000
N   -0.168046000000     0.000919000000    -0.000556000000
C   -0.701510000000    -1.102767000000     0.843658000000
H   -0.327659000000     0.638497000000    -1.995341000000
C   -0.702528000000     1.283260000000     0.533192000000
H   -0.319490000000    -1.123457000000    -1.768637000000
Ga   2.005934000000    -0.000214000000    -0.000063000000
H   -0.318730000000    -0.968407000000     1.857304000000
H   -0.325948000000    -2.045731000000     0.444742000000
H   -0.320354000000     2.094199000000    -0.089881000000
H   -0.327069000000     1.409505000000     1.549386000000
C    2.347045000000     1.193321000000    -1.591987000000
C    2.344029000000    -1.976358000000    -0.236899000000
C    2.345079000000     0.782242000000     1.829793000000
H    3.401894000000     1.475107000000    -1.625301000000
H    1.778903000000     2.127206000000    -1.551387000000
H    2.119602000000     0.703615000000    -2.541562000000
H    3.399400000000     0.669507000000     2.092246000000
H    1.775246000000     0.281633000000     2.617858000000
H    2.118524000000     1.849718000000     1.878874000000
H    3.397939000000    -2.148190000000    -0.466920000000
H    1.772882000000    -2.408108000000    -1.063798000000
H    2.117900000000    -2.552322000000     0.663378000000

2GaMe₃•hmta
N   -0.000011000000    -2.197224000000    -1.211386000000
N    0.000045000000    -2.198170000000     1.210774000000
N    1.214436000000    -0.482138000000     0.000387000000
C    1.181533000000    -1.351671000000     1.206145000000
C    1.185745000000    -1.357000000000    -1.201824000000
C    0.000028000000    -3.023086000000    -0.000450000000
H    2.082884000000    -1.966182000000     1.204393000000
H    2.081819000000    -1.977230000000    -1.190628000000
H    0.888060000000    -3.655856000000    -0.000716000000
C   -1.185775000000    -1.357031000000    -1.201775000000
Ga   3.007947000000     0.789932000000    -0.000335000000
H    1.187513000000    -0.711397000000     2.088603000000
H    1.203195000000    -0.719399000000    -2.087399000000
H   -0.887986000000    -3.655879000000    -0.000675000000
N   -1.214436000000    -0.482174000000     0.000423000000
C   -0.000010000000     0.352249000000    -0.008746000000
H   -2.081834000000    -1.977281000000    -1.190538000000
C   -1.181468000000    -1.351700000000     1.206184000000
H   -1.203282000000    -0.719433000000    -2.087350000000
Ga  -3.007952000000     0.789907000000    -0.000328000000
H   -0.000009000000     0.997069000000     0.872516000000
H   -0.000027000000     0.973226000000    -0.904435000000
H   -2.082797000000    -1.966240000000     1.204464000000
H   -1.187436000000    -0.711426000000     2.088643000000
C   -4.374047000000    -0.598885000000    -0.522743000000
C   -2.439438000000     2.121773000000    -1.402387000000
C   -2.969995000000     1.382971000000     1.926387000000
C    2.969999000000     1.382968000000     1.926388000000
C    2.439430000000     2.121771000000    -1.402414000000
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C	4.374005000000	-0.598909000000	-0.522730000000
H	-5.380358000000	-0.201479000000	-0.372936000000
H	-4.309817000000	-1.508204000000	0.081818000000
H	-4.301310000000	-0.887809000000	-1.573623000000
H	-3.676668000000	2.202653000000	2.073841000000
H	-1.992050000000	1.761692000000	2.237390000000
H	-3.258236000000	0.588617000000	2.618519000000
H	-3.290465000000	2.744031000000	-1.687993000000
H	-2.083051000000	1.647988000000	-2.321582000000
H	-1.657581000000	2.798752000000	-1.050377000000
H	4.309560000000	-1.508315000000	0.081681000000
H	5.380038000000	-0.201648000000	-0.372691000000
H	4.301403000000	-0.887674000000	-1.573664000000
H	1.992024000000	1.761565000000	2.237448000000
H	3.676578000000	2.202735000000	2.073819000000
H	3.258372000000	0.588634000000	2.618489000000
H	1.657464000000	2.798654000000	-1.050461000000
H	2.083167000000	1.647942000000	-2.321635000000
H	3.290402000000	2.744124000000	-1.687958000000

3GaMe₃•hmta

N	-0.000906000000	-0.001424000000	-2.378127000000
N	-1.150897000000	-0.795987000000	-0.401778000000
N	1.264937000000	-0.601093000000	-0.404323000000
C	0.112376000000	-1.379729000000	0.081092000000
C	1.238333000000	-0.584487000000	-1.889423000000
C	-1.124483000000	-0.782617000000	-1.887311000000
H	0.193375000000	-2.404829000000	-0.281191000000
H	1.336063000000	-1.611349000000	-2.243623000000
H	-1.045389000000	-1.811856000000	-2.236098000000
C	-0.106286000000	1.363578000000	-1.888610000000
Ga	-2.876553000000	-1.982582000000	0.344628000000
Ga	3.157378000000	-1.495889000000	0.345034000000
H	0.115081000000	-1.382940000000	1.171736000000
H	2.089799000000	-0.001477000000	-2.239249000000
H	-2.063234000000	-0.354485000000	-2.240830000000
N	-0.111769000000	1.393694000000	-0.403336000000
C	1.134905000000	0.781467000000	0.087116000000
H	-1.031973000000	1.819615000000	-2.241666000000
C	-1.253108000000	0.594126000000	0.074213000000
H	0.740620000000	1.952894000000	-2.238903000000
Ga	-0.282006000000	3.480264000000	0.345199000000
H	1.127699000000	0.775672000000	1.176698000000
H	1.985381000000	1.368859000000	-0.263086000000
H	-2.177429000000	1.032366000000	-0.299961000000
H	-1.268024000000	0.602290000000	1.165839000000
C	-2.244354000000	3.751148000000	-0.019915000000
C	1.041403000000	4.341463000000	-0.906275000000
C	0.294955000000	3.144279000000	2.245075000000
C	3.042711000000	-0.844003000000	2.246585000000
C	4.429749000000	-0.557147000000	-0.903739000000
C	2.723647000000	-3.428184000000	-0.024310000000
C	-4.326091000000	-0.633785000000	-0.025360000000
C	-2.258147000000	-2.213178000000	2.247517000000

C	-2.702512000000	-3.556081000000	-0.901024000000
H	-3.348494000000	-4.368100000000	-0.560140000000
H	-1.688359000000	-3.964964000000	-0.931938000000
H	-3.003902000000	-3.321690000000	-1.924351000000
H	-1.948029000000	-1.273770000000	2.714468000000
H	-1.433544000000	-2.923566000000	2.340434000000
H	-3.077625000000	-2.600245000000	2.856968000000
H	-4.296505000000	0.218236000000	0.657683000000
H	-5.305230000000	-1.101888000000	0.097244000000
H	-4.298296000000	-0.245840000000	-1.047721000000
H	-2.500196000000	4.805862000000	0.102494000000
H	-2.884471000000	3.190049000000	0.664753000000
H	-2.529442000000	3.483733000000	-1.041570000000
H	0.092799000000	4.028212000000	2.853854000000
H	1.364274000000	2.938775000000	2.333115000000
H	-0.245376000000	2.318395000000	2.716909000000
H	1.265741000000	5.354267000000	-0.564597000000
H	0.662899000000	4.429284000000	-1.927062000000
H	1.998518000000	3.813254000000	-0.945041000000
H	1.984130000000	-3.835008000000	0.669097000000
H	3.624905000000	-4.035439000000	0.084342000000
H	2.361263000000	-3.598263000000	-1.042310000000
H	3.223540000000	0.229376000000	2.339150000000
H	3.799999000000	-1.344439000000	2.853972000000
H	2.079691000000	-1.064477000000	2.716346000000
H	4.270948000000	0.524496000000	-0.941724000000
H	4.380919000000	-0.941368000000	-1.924990000000
H	5.456368000000	-0.702642000000	-0.560598000000

4GaMe₃•hmta

31	-2.126971000	-2.151401000	-2.176616000
7	-0.843565000	-0.855801000	-0.865615000
7	0.838027000	-0.854222000	0.873395000
7	0.872210000	0.849513000	-0.843420000
6	1.695018000	-0.011836000	0.022484000
6	0.028223000	-0.006185000	-1.694520000
6	-0.012318000	-1.694845000	0.013472000
1	2.321888000	-0.650378000	-0.598310000
1	0.666330000	-0.638113000	-2.312429000
1	0.619780000	-2.341784000	-0.596979000
6	-1.694989000	0.011818000	-0.034374000
31	2.108084000	-2.153603000	2.192157000
31	2.198400000	2.135025000	-2.120852000
1	2.329240000	0.612139000	0.654241000
1	-0.589347000	0.621318000	-2.337238000
1	-0.658447000	-2.309224000	0.638960000
7	-0.866786000	0.860917000	0.838217000
6	0.012073000	1.695107000	0.000990000
1	-2.349650000	-0.607480000	0.580929000
6	-0.028567000	0.006672000	1.695960000
1	-2.301078000	0.645211000	-0.680653000
31	-2.179638000	2.169852000	2.104546000
1	0.636938000	2.314091000	0.643330000
1	-0.598938000	2.337224000	-0.635309000

1	-0.668754000	-0.618858000	2.318245000
1	0.590562000	0.637211000	2.334264000
6	-2.750932000	0.765038000	3.428137000
6	-3.476559000	2.706274000	0.662024000
6	-0.767654000	3.489976000	2.664381000
6	-2.689510000	-3.469779000	-0.763686000
6	-0.695842000	-2.702545000	-3.480305000
6	-3.437633000	-0.732306000	-2.739999000
6	2.712285000	3.466003000	-0.701332000
6	0.812351000	2.673961000	-3.477421000
6	3.527572000	0.712309000	-2.629122000
6	0.679825000	-3.473670000	2.708811000
6	2.630958000	-0.739890000	3.526290000
6	3.455972000	-2.695959000	0.799231000
1	4.079348000	-3.504933000	1.186143000
1	4.131272000	-1.883216000	0.522295000
1	2.995257000	-3.077898000	-0.116482000
1	1.809757000	-0.459398000	4.189637000
1	3.013284000	0.171237000	3.056784000
1	3.435692000	-1.114288000	4.162622000
1	-0.232813000	-2.993983000	3.074516000
1	1.039532000	-4.104633000	3.524414000
1	0.404193000	-4.143277000	1.890917000
1	-3.578298000	1.143702000	4.032117000
1	-1.954360000	0.489734000	4.122988000
1	-3.115827000	-0.149750000	2.951916000
1	-1.154477000	4.125352000	3.464009000
1	-0.461946000	4.155396000	1.853838000
1	0.130616000	3.010362000	3.064249000
1	-4.110303000	3.519943000	1.021265000
1	-4.144589000	1.893761000	0.367330000
1	-2.982975000	3.080386000	-0.239691000
1	4.177290000	0.421324000	-1.800591000
1	4.178421000	1.083916000	-3.423509000
1	3.054585000	-0.192821000	-3.021255000
1	1.894540000	4.139481000	-0.434915000
1	3.530385000	4.092431000	-1.063333000
1	3.073369000	2.994601000	0.217404000
1	-0.107955000	3.052454000	-3.022983000
1	0.544821000	1.860453000	-4.155489000
1	1.200766000	3.484948000	-4.097243000
1	0.208806000	-3.074996000	-2.990786000
1	-0.406136000	-1.895681000	-4.157169000
1	-1.062267000	-3.520540000	-4.104260000
1	-3.085171000	-2.989881000	0.136227000
1	-1.880431000	-4.138109000	-0.460279000
1	-3.492263000	-4.102213000	-1.148814000
1	-4.116216000	-0.437297000	-1.936379000
1	-4.059767000	-1.108738000	-3.554850000
1	-2.951637000	0.171049000	-3.120138000

GaCl₃•hmta
N	0.000000000000	1.399058000000	-2.479069000000
N	-1.211620000000	-0.699529000000	-2.479069000000

N	1.211620000000	-0.699529000000	-2.479069000000
C	0.000000000000	-1.374234000000	-2.953198000000
C	1.190122000000	0.687117000000	-2.953198000000
C	-1.190122000000	0.687117000000	-2.953198000000
H	0.000000000000	-1.377319000000	-4.043442000000
H	1.192793000000	0.688660000000	-4.043442000000
H	-1.192793000000	0.688660000000	-4.043442000000
C	0.000000000000	1.404598000000	-1.034534000000
H	0.000000000000	-2.404614000000	-2.594849000000
H	2.082457000000	1.202307000000	-2.594849000000
H	-2.082457000000	1.202307000000	-2.594849000000
N	0.000000000000	0.000000000000	-0.489924000000
C	1.216417000000	-0.702299000000	-1.034534000000
H	-0.890435000000	1.906191000000	-0.652820000000
C	-1.216417000000	-0.702299000000	-1.034534000000
H	0.890435000000	1.906191000000	-0.652820000000
Ga	0.000000000000	0.000000000000	1.559033000000
H	1.205592000000	-1.724234000000	-0.652820000000
H	2.096027000000	-0.181956000000	-0.652820000000
H	-2.096027000000	-0.181956000000	-0.652820000000
H	-1.205592000000	-1.724234000000	-0.652820000000
Cl	0.000000000000	-2.129347000000	2.015115000000
Cl	1.844069000000	1.064674000000	2.015115000000
Cl	-1.844069000000	1.064674000000	2.015115000000

2GaCl₃•hmta

Ga	0.000000000000	2.932673000000	-0.554135000000
N	0.000000000000	1.216350000000	0.628382000000
N	1.205492000000	0.000000000000	2.343113000000
N	-1.205492000000	0.000000000000	2.343113000000
C	0.000000000000	0.000000000000	3.175405000000
C	-1.217615000000	1.182196000000	1.512194000000
C	1.217615000000	1.182196000000	1.512194000000
H	0.000000000000	0.888519000000	3.806193000000
H	-1.204185000000	2.081873000000	2.127084000000
H	1.204185000000	2.081873000000	2.127084000000
C	0.000000000000	0.000000000000	-0.218270000000
H	0.000000000000	-0.888519000000	3.806193000000
H	-2.097649000000	1.192033000000	0.868183000000
H	2.097649000000	1.192033000000	0.868183000000
N	0.000000000000	-1.216350000000	0.628382000000
C	-1.217615000000	-1.182196000000	1.512194000000
H	0.892366000000	0.000000000000	-0.847142000000
C	1.217615000000	-1.182196000000	1.512194000000
H	-0.892366000000	0.000000000000	-0.847142000000
Ga	0.000000000000	-2.932673000000	-0.554135000000
H	-1.204185000000	-2.081873000000	2.127084000000
H	-2.097649000000	-1.192033000000	0.868183000000
H	2.097649000000	-1.192033000000	0.868183000000
H	1.204185000000	-2.081873000000	2.127084000000
Cl	0.000000000000	4.472094000000	0.980288000000
Cl	1.850302000000	2.666403000000	-1.654544000000
Cl	-1.850302000000	2.666403000000	-1.654544000000
Cl	-1.850302000000	-2.666403000000	-1.654544000000

| Cl | 0.000000000000 | -4.472094000000 | 0.980288000000 |
| Cl | 1.850302000000 | -2.666403000000 | -1.654544000000 |

3GaCl₃•hmta

Ga	2.949606000000	1.702956000000	-0.227842000000
N	1.212861000000	0.700246000000	0.456138000000
N	0.000000000000	0.000000000000	2.422618000000
N	-1.212861000000	0.700246000000	0.456138000000
C	-1.185633000000	0.684525000000	1.958115000000
C	0.000000000000	1.393405000000	-0.035834000000
C	1.185633000000	0.684525000000	1.958115000000
H	-1.193088000000	1.718185000000	2.302634000000
H	0.000000000000	2.420242000000	0.332016000000
H	1.193088000000	1.718185000000	2.302634000000
C	1.206724000000	-0.696702000000	-0.035834000000
Ga	-2.949606000000	1.702956000000	-0.227842000000
H	-2.084536000000	0.174151000000	2.302634000000
H	0.000000000000	1.390581000000	-1.127344000000
H	2.084536000000	0.174151000000	2.302634000000
N	0.000000000000	-1.400491000000	0.456138000000
C	-1.206724000000	-0.696702000000	-0.035834000000
H	2.095991000000	-1.210121000000	0.332016000000
C	0.000000000000	-1.369051000000	1.958115000000
H	1.204278000000	-0.695290000000	-1.127344000000
Ga	0.000000000000	-3.405912000000	-0.227842000000
H	-2.095991000000	-1.210121000000	0.332016000000
H	-1.204278000000	-0.695290000000	-1.127344000000
H	0.891448000000	-1.892337000000	2.302634000000
H	-0.891448000000	-1.892337000000	2.302634000000
Cl	2.614567000000	3.642668000000	0.677366000000
Cl	4.461926000000	0.442947000000	0.677366000000
Cl	2.648205000000	1.528942000000	-2.362160000000
Cl	0.000000000000	-3.057884000000	-2.362160000000
Cl	-1.847360000000	-4.085615000000	0.677366000000
Cl	1.847360000000	-4.085615000000	0.677366000000
Cl	-2.648205000000	1.528942000000	-2.362160000000
Cl	-4.461926000000	0.442947000000	0.677366000000
Cl	-2.614567000000	3.642668000000	0.677366000000

4GaCl₃•hmta

Ga	2.098248000000	-2.098248000000	2.098248000000
N	0.855101000000	-0.855101000000	0.855101000000
N	-0.855101000000	0.855101000000	0.855101000000
N	0.855101000000	0.855101000000	-0.855101000000
C	0.000000000000	1.708257000000	0.000000000000
C	1.708257000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.708257000000
H	0.631954000000	2.333451000000	0.631954000000
H	2.333451000000	0.631954000000	0.631954000000
H	0.631954000000	0.631954000000	2.333451000000
C	0.000000000000	-1.708257000000	0.000000000000
Ga	-2.098248000000	2.098248000000	2.098248000000
Ga	2.098248000000	2.098248000000	-2.098248000000
H	-0.631954000000	2.333451000000	-0.631954000000

H	2.333451000000	-0.631954000000	-0.631954000000
H	-0.631954000000	-0.631954000000	2.333451000000
N	-0.855101000000	-0.855101000000	-0.855101000000
C	0.000000000000	0.000000000000	-1.708257000000
H	-0.631954000000	-2.333451000000	0.631954000000
C	-1.708257000000	0.000000000000	0.000000000000
H	0.631954000000	-2.333451000000	-0.631954000000
Ga	-2.098248000000	-2.098248000000	-2.098248000000
H	-0.631954000000	0.631954000000	-2.333451000000
H	0.631954000000	-0.631954000000	-2.333451000000
H	-2.333451000000	-0.631954000000	0.631954000000
H	-2.333451000000	0.631954000000	-0.631954000000
Cl	3.151660000000	-0.532915000000	3.151660000000
Cl	0.532915000000	-3.151660000000	3.151660000000
Cl	3.151660000000	-3.151660000000	0.532915000000
Cl	-0.532915000000	-3.151660000000	-3.151660000000
Cl	-3.151660000000	-0.532915000000	-3.151660000000
Cl	-3.151660000000	-3.151660000000	-0.532915000000
Cl	3.151660000000	0.532915000000	-3.151660000000
Cl	0.532915000000	3.151660000000	-3.151660000000
Cl	-0.532915000000	3.151660000000	3.151660000000
Cl	-3.151660000000	0.532915000000	3.151660000000
Cl	-3.151660000000	3.151660000000	0.532915000000
Cl	3.151660000000	3.151660000000	-0.532915000000

AlBr₃·pyz

Br	1.051302000000	-1.074228000000	1.913294000000
Br	1.051302000000	-1.074228000000	-1.913294000000
Br	1.051302000000	2.284053000000	0.000000000000
Al	0.562756000000	0.060580000000	0.000000000000
N	-1.432377000000	-0.005600000000	0.000000000000
N	-4.180804000000	-0.256664000000	0.000000000000
C	-2.214227000000	1.074096000000	0.000000000000
C	-3.594735000000	0.931653000000	0.000000000000
C	-3.388563000000	-1.322636000000	0.000000000000
C	-2.009075000000	-1.211523000000	0.000000000000
H	-1.723787000000	2.038221000000	0.000000000000
H	-4.232934000000	1.806131000000	0.000000000000
H	-3.859219000000	-2.297325000000	0.000000000000
H	-1.354743000000	-2.074169000000	0.000000000000

pyz·AlBr₃·pyz

Br	0.221204000000	-1.999992000000	1.255016000000
Br	-0.000073000000	0.000419000000	-2.274783000000
Br	-0.221142000000	1.999626000000	1.255726000000
Al	0.000000000000	0.000011000000	0.068994000000
N	-2.133742000000	-0.121402000000	0.000179000000
N	-4.903833000000	-0.071860000000	-0.216487000000
C	-2.766771000000	0.883130000000	-0.613451000000
C	-4.145852000000	0.899094000000	-0.715730000000
C	-4.268473000000	-1.062773000000	0.388401000000
C	-2.883694000000	-1.098309000000	0.503222000000
H	-2.156413000000	1.675760000000	-1.023629000000
H	-4.646840000000	1.718788000000	-1.214743000000

H	-4.867558000000	-1.864555000000	0.801900000000
H	-2.372818000000	-1.910367000000	0.998727000000
N	2.133750000000	0.121398000000	0.000141000000
C	2.766757000000	-0.883167000000	-0.613459000000
H	2.156381000000	-1.675799000000	-1.023606000000
C	4.145837000000	-0.899168000000	-0.715737000000
H	4.646806000000	-1.718886000000	-1.214729000000
N	4.903842000000	0.071779000000	-0.216517000000
C	4.268507000000	1.062712000000	0.388365000000
H	4.867613000000	1.864481000000	0.801860000000
C	2.883730000000	1.098281000000	0.503190000000
H	2.372877000000	1.910352000000	0.998698000000

AlBr₃·pyz·AlBr₃

Br	3.939008000000	1.463854000000	-1.182574000000
Br	3.958740000000	-2.208880000000	0.057903000000
Br	3.484040000000	0.719182000000	2.549608000000
Al	3.369136000000	-0.046430000000	0.414656000000
N	1.355864000000	-0.067985000000	0.160494000000
C	0.660568000000	-1.157824000000	-0.163170000000
H	1.210999000000	-2.080319000000	-0.289796000000
C	0.711827000000	1.087516000000	0.325321000000
H	1.301915000000	1.956089000000	0.588290000000
Br	-3.939008000000	-1.463854000000	1.182574000000
Br	-3.958740000000	2.208880000000	-0.057903000000
Br	-3.484040000000	-0.719182000000	-2.549608000000
Al	-3.369136000000	0.046430000000	-0.414656000000
N	-1.355864000000	0.067985000000	-0.160494000000
C	-0.660568000000	1.157824000000	0.163170000000
H	-1.210999000000	2.080319000000	0.289796000000
C	-0.711827000000	-1.087516000000	-0.325321000000
H	-1.301915000000	-1.956089000000	-0.588290000000

GaCl₃·pyz

Cl	1.107349000000	1.364152000000	1.824877000000
Cl	1.107349000000	1.364152000000	-1.824877000000
Cl	-2.112195000000	1.508323000000	0.000000000000
Ga	-0.004581000000	0.994552000000	0.000000000000
N	-0.063387000000	-1.077458000000	0.000000000000
N	-0.013965000000	-3.831369000000	0.000000000000
C	-1.198179000000	-1.773569000000	0.000000000000
C	-1.157543000000	-3.160835000000	0.000000000000
C	1.107349000000	-3.120383000000	0.000000000000
C	1.096758000000	-1.735290000000	0.000000000000
H	-2.122380000000	-1.210402000000	0.000000000000
H	-2.075286000000	-3.735173000000	0.000000000000
H	2.044434000000	-3.662267000000	0.000000000000
H	2.003822000000	-1.143674000000	0.000000000000

pyz·GaCl₃·pyz

Cl	0.145785000000	-1.927196000000	1.126813000000
Cl	-0.000012000000	-0.000271000000	-2.161645000000
Cl	-0.145789000000	1.927745000000	1.126392000000
Ga	0.000002000000	0.000042000000	0.051483000000

N	-2.207841000000	-0.080606000000	0.023315000000
N	-4.972325000000	0.022200000000	-0.098110000000
C	-2.831452000000	0.898220000000	-0.631155000000
C	-4.214647000000	0.940960000000	-0.686644000000
C	-4.339433000000	-0.944743000000	0.550064000000
C	-2.953142000000	-1.006495000000	0.617619000000
H	-2.212867000000	1.645303000000	-1.111237000000
H	-4.718398000000	1.737278000000	-1.219966000000
H	-4.944205000000	-1.700823000000	1.035286000000
H	-2.433211000000	-1.794591000000	1.144277000000
N	2.207847000000	0.080571000000	0.023276000000
C	2.831401000000	-0.898536000000	-0.630830000000
H	2.212772000000	-1.645763000000	-1.110631000000
C	4.214595000000	-0.941379000000	-0.686305000000
H	4.718298000000	-1.737926000000	-1.219332000000
N	4.972327000000	-0.022447000000	-0.098113000000
C	4.339492000000	0.944771000000	0.549708000000
H	4.944310000000	1.700988000000	1.034659000000
C	2.953206000000	1.006625000000	0.617250000000
H	2.433326000000	1.794940000000	1.143628000000

GaCl$_3$·pyz·GaCl$_3$

Cl	3.973631000000	1.263385000000	-1.219112000000
Cl	3.886699000000	-2.146296000000	0.224543000000
Cl	3.548687000000	0.854532000000	2.391747000000
Ga	3.446141000000	-0.038175000000	0.423419000000
N	1.348992000000	-0.056509000000	0.179958000000
C	0.687948000000	-1.124697000000	-0.259145000000
H	1.263369000000	-2.019598000000	-0.457642000000
C	0.683512000000	1.066053000000	0.441854000000
H	1.252870000000	1.913138000000	0.803155000000
Cl	-3.973631000000	-1.263385000000	1.219112000000
Cl	-3.886699000000	2.146296000000	-0.224543000000
Cl	-3.548687000000	-0.854532000000	-2.391747000000
Ga	-3.446141000000	0.038175000000	-0.423419000000
N	-1.348992000000	0.056509000000	-0.179958000000
C	-0.687948000000	1.124697000000	0.259145000000
H	-1.263369000000	2.019598000000	0.457642000000
C	-0.683512000000	-1.066053000000	-0.441854000000
H	-1.252870000000	-1.913138000000	-0.803155000000

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