Synthesis and Characterization of $(pyNO^{-})_2GaCl$: A Redox-Active Gallium Complex

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Electronic Supplementary Information

Figure S1. ^{1}H NMR spectrum of $(pyNO^{-})_2GaCl$ (**1**).

Figure S2. ^{13}C NMR spectrum of $(pyNO^{-})_2GaCl$ (**1**).

Table S1. Summary of Structure Determination of $(pyNO^{-})_2GaCl$ (**1**).

Table S2. Summary of Structure Determination of $\{(pyNO^{-})_2In\}\{(pyNO^{-})_2InCl_2\}$ (**2**).

Figure S3. Solid state structure of $\{(pyNO^{-})_2In\}\{(pyNO^{-})_2InCl_2\}$ (**2**).

Table S3. Optimized coordinates of $(pyNO^{-})_2GaCl$ (**1**).

Full Gaussian '09 Reference.

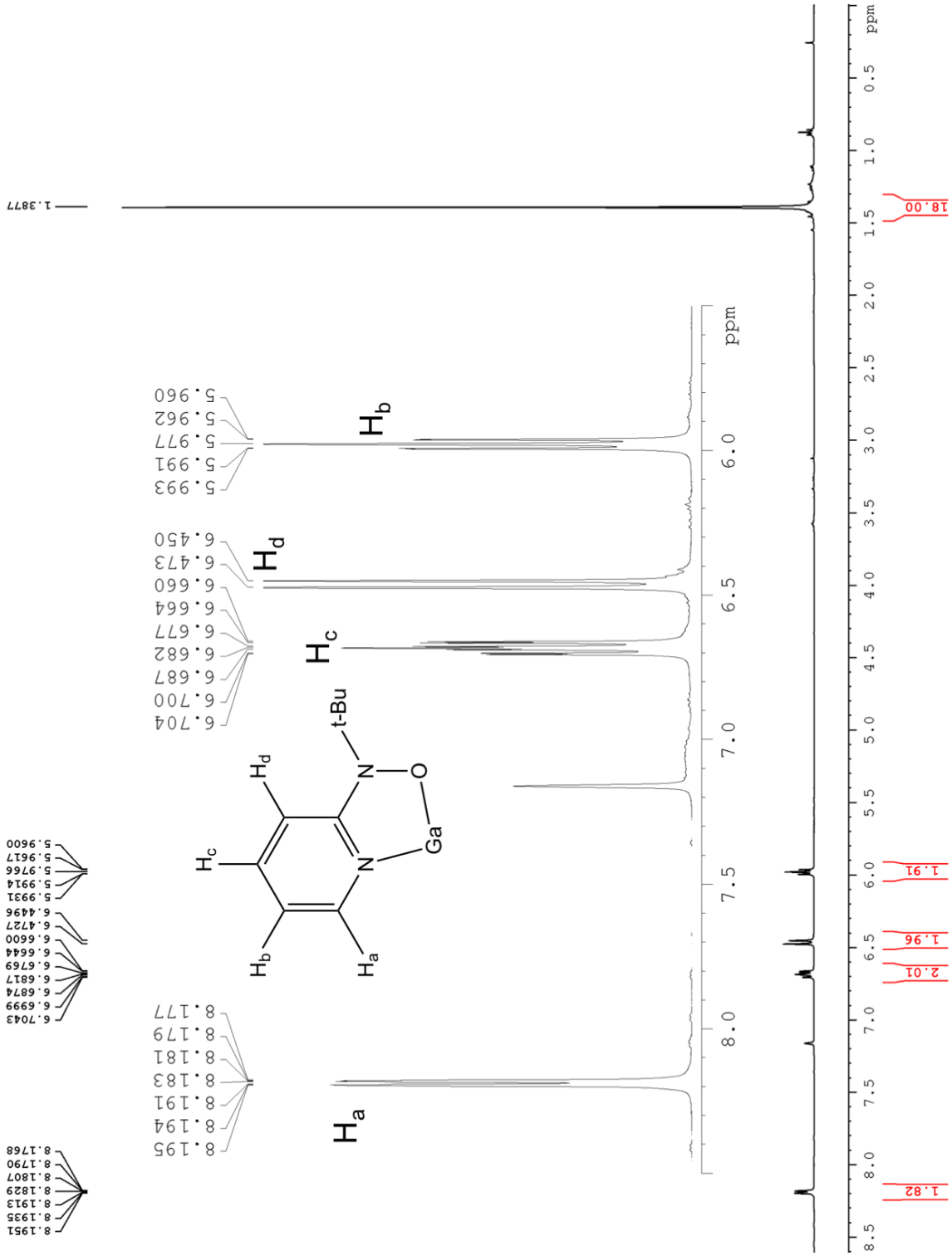


Figure S1. ^{1}H NMR spectrum of $(pyNO^-)_2GaCl$ (**1**). Taken in C_6D_6 at 25 °C.

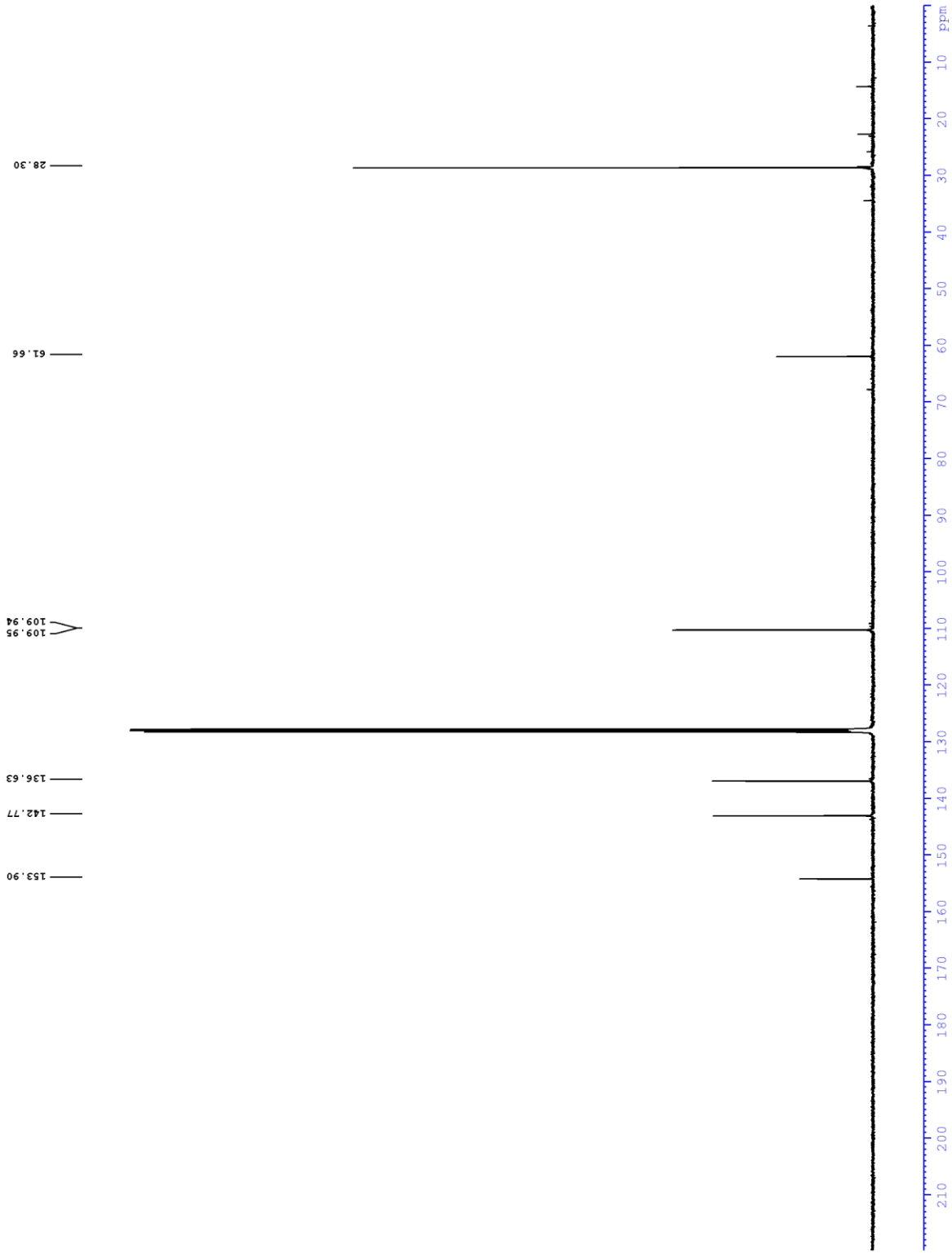


Figure S2. ^{13}C NMR spectrum of $(pyNO^{-})_2GaCl$ (**1**). Taken in C_6D_6 at 25 °C.

Table S1. Summary of Structure Determination of $(pyNO^{-})_2GaCl$ (1).

Empirical formula	$C_{18}H_{26}ClGaN_4O_2$
Formula weight	435.60
Temperature/K	100
Crystal system	orthorhombic
Space group	$Pna2_1$
a	17.1517(9)Å
b	13.0663(7)Å
c	8.8556(5)Å
Volume	1984.62(19)$Å^3$
Z	4
d_{calc}	1.458 g/cm^3
μ	1.541 mm^{-1}
F(000)	904.0
Crystal size, mm	0.23 × 0.18 × 0.15
2θ range for data collection	6.044 - 55.004°
Index ranges	$-22 \leq h \leq 22$, $-16 \leq k \leq 13$, $-11 \leq l \leq 11$
Reflections collected	24139
Independent reflections	4528[R(int) = 0.0290]
Data/restraints/parameters	4528/1/241
Goodness-of-fit on F^2	1.091
Final R indexes [I>=2σ (I)]	R_1 = 0.0226, wR_2 = 0.0481
Final R indexes [all data]	R_1 = 0.0260, wR_2 = 0.0491
Largest diff. peak/hole	0.21/-0.34 $eÅ^{-3}$
Flack parameter	0.042(4)

Table S2. Summary of Structure Determination of $\{(pyNO^{-})_2In\}\{(pyNO^{-})_2InCl_2\}$ (**2**).

Empirical formula	$C_{40}H_{62}N_8O_5Cl_2In_2$
Formula weight	1035.51
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a	16.9046(13)Å
b	12.8148(9)Å
c	21.4132(17)Å
β	98.458(2)°
Volume	4588.3(6)Å^3
Z	4
d_{calc}	1.499 g/cm^3
μ	1.171 mm^{-1}
F(000)	2120.0
Crystal size, mm	0.18 × 0.18 × 0.18
2θ range for data collection	2.872 - 55.044°
Index ranges	$-21 \leq h \leq 21$, $-14 \leq k \leq 16$, $-27 \leq l \leq 27$
Reflections collected	127236
Independent reflections	10557[R(int) = 0.0241]
Data/restraints/parameters	10557/174/576
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0253, wR_2 = 0.0574
Final R indexes [all data]	R_1 = 0.0290, wR_2 = 0.0600
Largest diff. peak/hole	1.54/-0.98 eÅ^{-3}

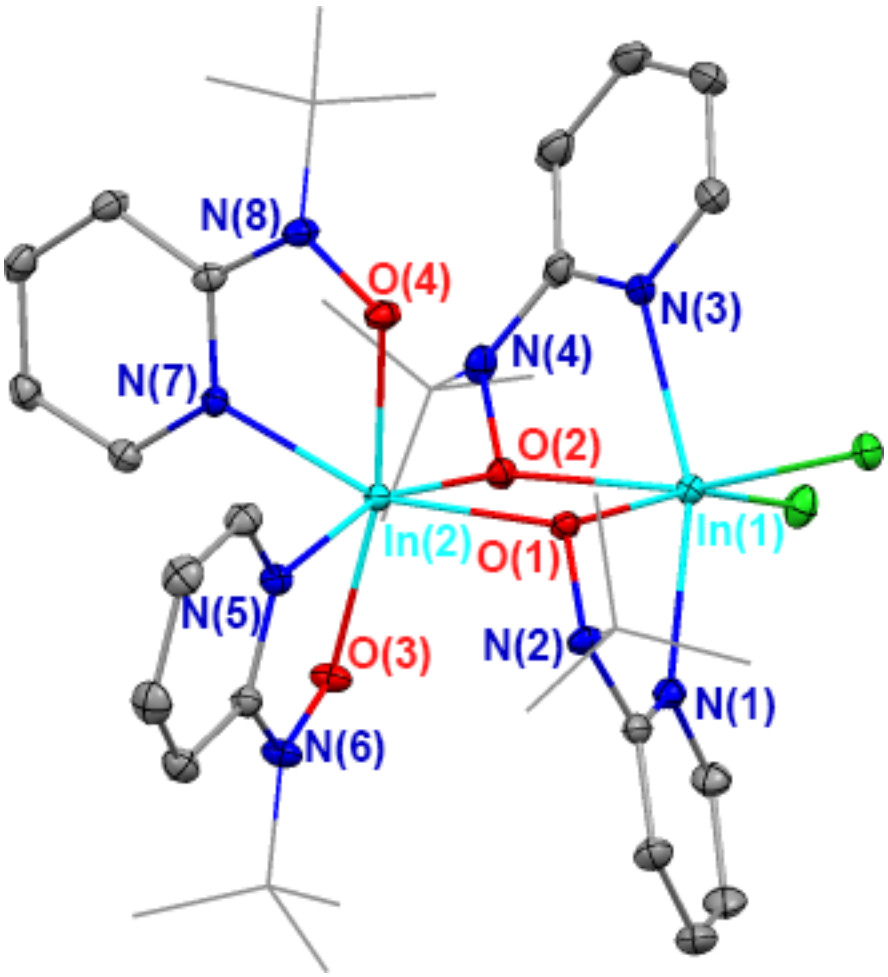
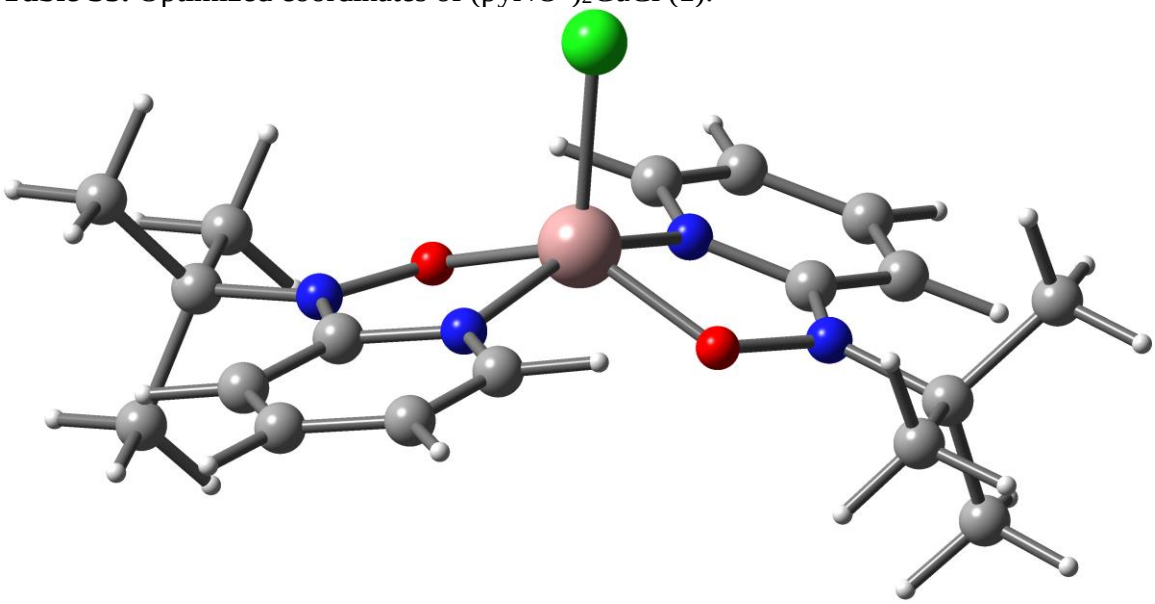


Figure S3. Solid state structure of $\{(pyNO^{-})_2In\}\{(pyNO^{-})_2InCl_2\}$ (**2**). Ellipsoids are projected at 30% probability and H atoms are omitted for clarity.

Selected bond distances (Å): In(1)-Cl(1), 2.4438(6); In(1)-Cl(2), 2.4605(6); In(1)-O(1), 2.2063(15); In(1)-O(2), 2.2086(14); In(1)-N(1), 2.2242(18); In(1)-N(3), 2.2308(18); In(2)-O(1), 2.1940(14); In(2)-O(2), 2.2114(15); In(2)-O(3), 2.0978(15); In(2)-O(4), 2.1064(15); In(2)-N(5), 2.2114(19); In(2)-N(7), 2.2155(17); O(1)-N(2), 1.410(2); O(2)-N(4), 1.408(2); O(3)-N(6), 1.386(2); O(4)-N(8), 1.383(2).

Selected bond angles (º): Cl(1)-In(1)-Cl(2), 99.09(2); O(1)-In(1)-Cl(1), 92.41(4); O(1)-In(1)-Cl(2), 163.01(4); O(1)-In(1)-O(2), 75.03(5); O(1)-In(1)-N(1), 70.69(6); O(1)-In(1)-N(3), 96.33(6); O(2)-In(1)-Cl(1), 159.10(4); O(2)-In(1)-Cl(2), 97.12(4); O(2)-In(1)-N(1), 91.94(6); O(2)-In(1)-N(3), 70.02(6); N(1)-In(1)-Cl(1), 99.69(5); N(1)-In(1)-Cl(2), 94.93(5); N(1)-In(1)-N(3), 160.35(7); N(3)-In(1)-Cl(1); 95.43(5); N(3)-In(1)-Cl(2), 94.99(5); O(1)-In(2)-O(2), 75.22(5); O(1)-In(2)-N(5), 97.00(6); O(1)-In(2)-N(7), 159.52(6); O(2)-In(2)-N(5), 162.53(6); O(2)-In(2)-N(7), 96.38(6); O(3)-In(2)-O(1), 101.47(6); O(3)-In(2)-O(2), 91.35(6); O(3)-In(2)-O(4), 166.97(6); O(3)-In(2)-N(5), 74.66(6); O(3)-In(2)-N(7), 97.32(6); O(4)-In(2)-O(1), 88.52(6); O(4)-In(2)-O(2), 99.35(6); O(4)-In(2)-N(5), 96.01(7); O(4)-In(2)-N(7), 74.24(6); N(5)-In(2)-N(7), 95.76(7).

Table S3. Optimized coordinates of $(pyNO^{-})_2GaCl$ (**1**).



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C	3.933278155	1.1801397214	-0.6114811658
C	2.709288382	0.4646541048	-0.3897878887
N	2.529665522	-0.8820434187	-0.4601449142
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Full Gaussian ’09 Reference:

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.