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Supporting Information for:

Cationic Indium Methyl Complexes Incorporating Aminotroponiminate Ligands

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I. NMR Data for Free Borate Anions and Lewis Bases in C_6D_5Cl

NMR Data for Free $B(C_6F_5)_4^-$ anion in C_6D_5Cl. **^{13}C NMR** (C_6D_5Cl) δ 148.9 (d, $^1J_{CF}$ = 238), 138.7 (d, $^1J_{CF}$ = 246), 136.9 (d, $^1J_{CF}$ = 245), 126.5 (br, C_{ipso}). **^{11}B NMR** (C_6D_5Cl) δ -16.4 (s). **^{19}F NMR** (C_6D_5Cl) δ -132.2 (d, $^3J_{FF}$ = 10.5, 8F, F_o), -162.7 (t, $^3J_{FF}$ = 21, 4F, F_p), -166.7 (t, $^3J_{FF}$ = 18.5, 8F, F_m).

NMR Data for $[NBu_3(CH_2Ph)][MeB(C_6F_5)_3]$ in C_6D_5Cl. **^1H NMR** (C_6D_5Cl): δ 7.23 (m, 3H), 6.92 (d, *J* = 6.8, 2H), 3.67 (s, 2H), 2.45 (m, 6H), 1.29 (m, 6H), 1.11 (br s, 3H, BMe), 1.05 (m, 6H), 0.79 (t, *J* = 7.3, 9H). **$^{13}C\{^1H\}$ NMR** (C_6D_5Cl): δ 149.1 (d, $^1J_{CF}$ = 240), 138.0 (d, $^1J_{CF}$ = 245), 136.9 (d, $^1J_{CF}$ =246), 131.8 (s, *o*-Ph or *m*-Ph overlapped with *p*-Ph), 130.0 (s, *o*- or *m*-Ph), 125.4 (s, *ipso*-Ph), 62.2 ($CH_2C_6H_5$), 58.0 (α-butyl), 23.8 (β-butyl), 19.6 (γ-butyl), 13.3 (δ-butyl), 11.4 (br s, BMe). **$^{11}B\{^1H\}$ NMR** (C_6D_5Cl): δ -14.6. **^{19}F NMR** (C_6D_5Cl): δ -132.3 (6F, *o*-C_6F_5), -164.5 (3F, *p*-C_6F_5), -167.1 (6F, *m*-C_6F_5).

NMR Data for NMe_2Ph in C_6D_5Cl. ^1H NMR (C_6D_5Cl): δ 2.65 (s, 6H, NMe), 6.61 (d, 2H, $^3J_{HH}$ = 8.3, *o*-Ph), 6.73 (t, 1H, $^3J_{HH}$ = 7.2, *p*-Ph), 7.20 (t, 2H, $^3J_{HH}$ = 7.7, *m*-Ph). ^{13}C NMR (C_6D_5Cl): δ 40.2 (d, $^1J_{CH}$ = 137, Me), 112.8 (d, $^1J_{CH}$ = 157, *o*-Ph, 116.8 (d, $^1J_{CH}$ = 160, *p*-Ph), 129.2 (d, $^1J_{CH}$ = 156, *m*-Ph), 150.8 (s, *ipso*-Ph).

NMR Data for MeCN in C_6D_5Cl. ^1H NMR (C_6D_5Cl): δ 1.37 (s). ^{13}C NMR (C_6D_5Cl): δ 1.5 (q, $^1J_{CH}$ = 136, *Me*CN), 116.3 (s, br, Me*C*N).

NMR Data for Me_2CO in C_6D_5Cl. ^1H NMR (C_6D_5Cl): δ 1.77 (s). ^{13}C NMR (C_6D_5Cl): δ 30.5 (q, $^1J_{CH}$ = 127, Me_2CO), 221.1 (s, *C*=O).

NMR Data for PMe_3 in C_6D_5Cl. ^1H NMR (C_6D_5Cl): δ 0.79 (d, $^3J_{HP}$ = 2.6) . ^{13}C NMR (C_6D_5Cl): δ 16.8 (q, $^1J_{CH}$ = 127). $^{31}P\{^1H\}$ NMR (C_6D_5Cl): δ -65.1 (s).

I. X-ray Crystallographic Analysis of (^{i}Pr$_2$-ATI)InCl$_2$ (**3**).

Crystallographic Experimental Section

Data Collection

A pale yellow air-sensitive crystal with approximate dimensions 0.45 x 0.42 x 0.31 mm^3 was selected under oil under ambient conditions and attached to the tip of a glass capillary. The crystal was mounted in a stream of cold nitrogen at 183(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 5.08 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° in a 6° range about ω with the exposure time of 10 seconds per frame. A total of 185 reflections was obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 8192 strong reflections from the actual data collection.

The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of 0.8 hemisphere to a resolution of 0.80 Å. A total of 18844 data were harvested by collecting two sets of frames with 0.4° scans in ω with an exposure time 10 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement [2]. A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen

atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. There are two independent molecules of the complex in the asymmetric unit. The final least-squares refinement of 333 parameters against 6472 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0260 and 0.0517, respectively. The final difference Fourier map was featureless.

The ORTEP diagrams were drawn with 30% probability ellipsoids.

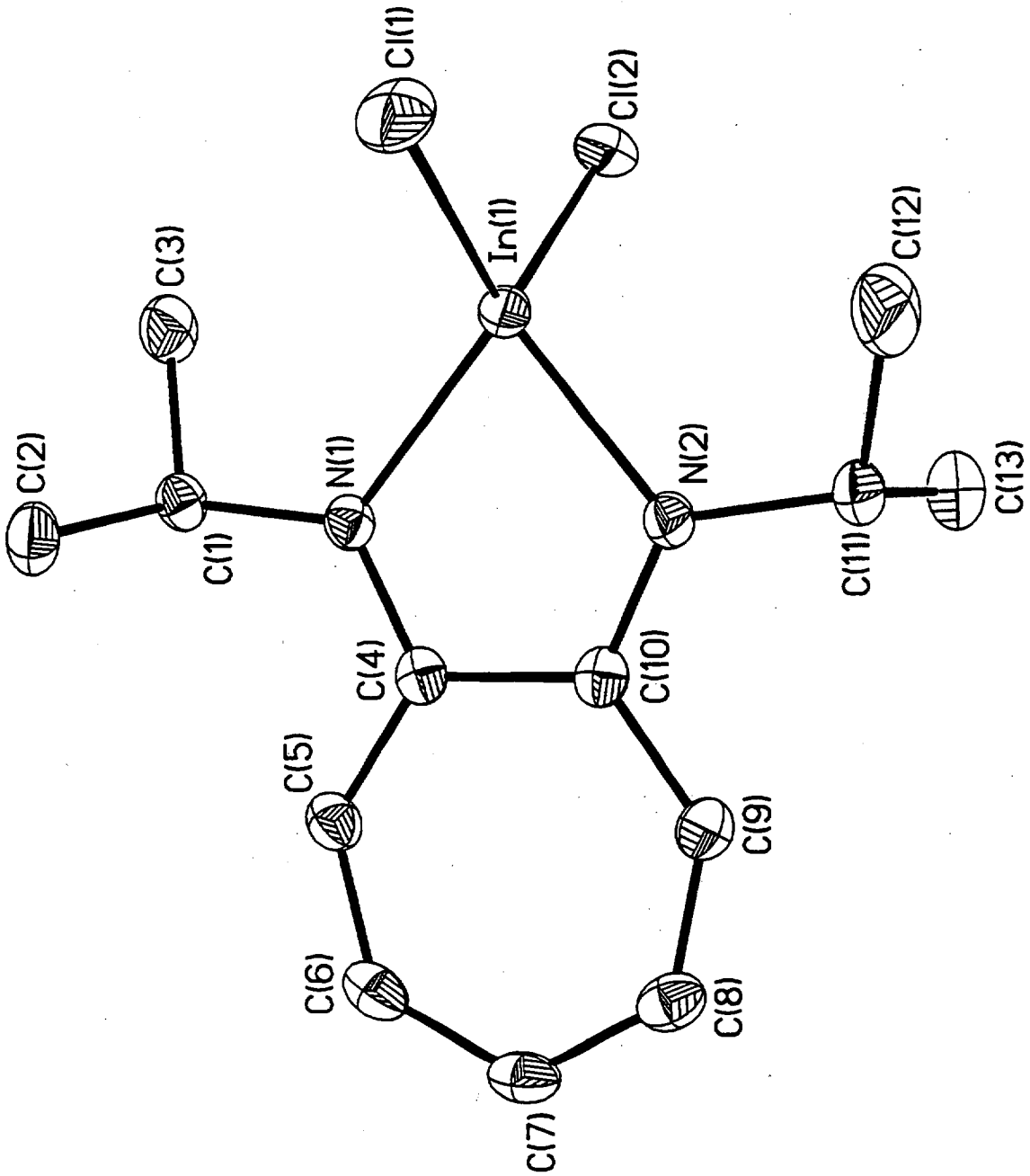
References

[1] Blessing, R.H. *Acta Cryst.* **1995**, *A51*, 33-38.

[2] All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).

Crystal data and structure refinement for **3**

Identification code	jor19	
Empirical formula	$C_{13}H_{19}Cl_2InN_2$	
Formula weight	389.02	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.8218(10) Å	α= 90°
	b = 16.5938(12) Å	β= 116.231(1)°
	c = 15.5339(11) Å	γ = 90°
Volume	3195.9(4) Å^3	
Z	8	
Density (calculated)	1.617 Mg/m^3	
Absorption coefficient	1.799 mm^{-1}	
F(000)	1552	
Crystal size	0.45 x 0.42 x 0.31 mm^3	
Theta range for data collection	1.64 to 26.37°.	
Index ranges	-17<=h<=15, 0<=k<=20, 0<=l<=19	
Reflections collected	18844	
Independent reflections	6472 [R(int) = 0.0230]	
Completeness to theta = 26.37°	99.0 %	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.6055 and 0.4982	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6472 / 0 / 333	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0260, wR2 = 0.0517	
R indices (all data)	R1 = 0.0412, wR2 = 0.0550	
Largest diff. peak and hole	0.598 and -0.498 e.Å^{-3}	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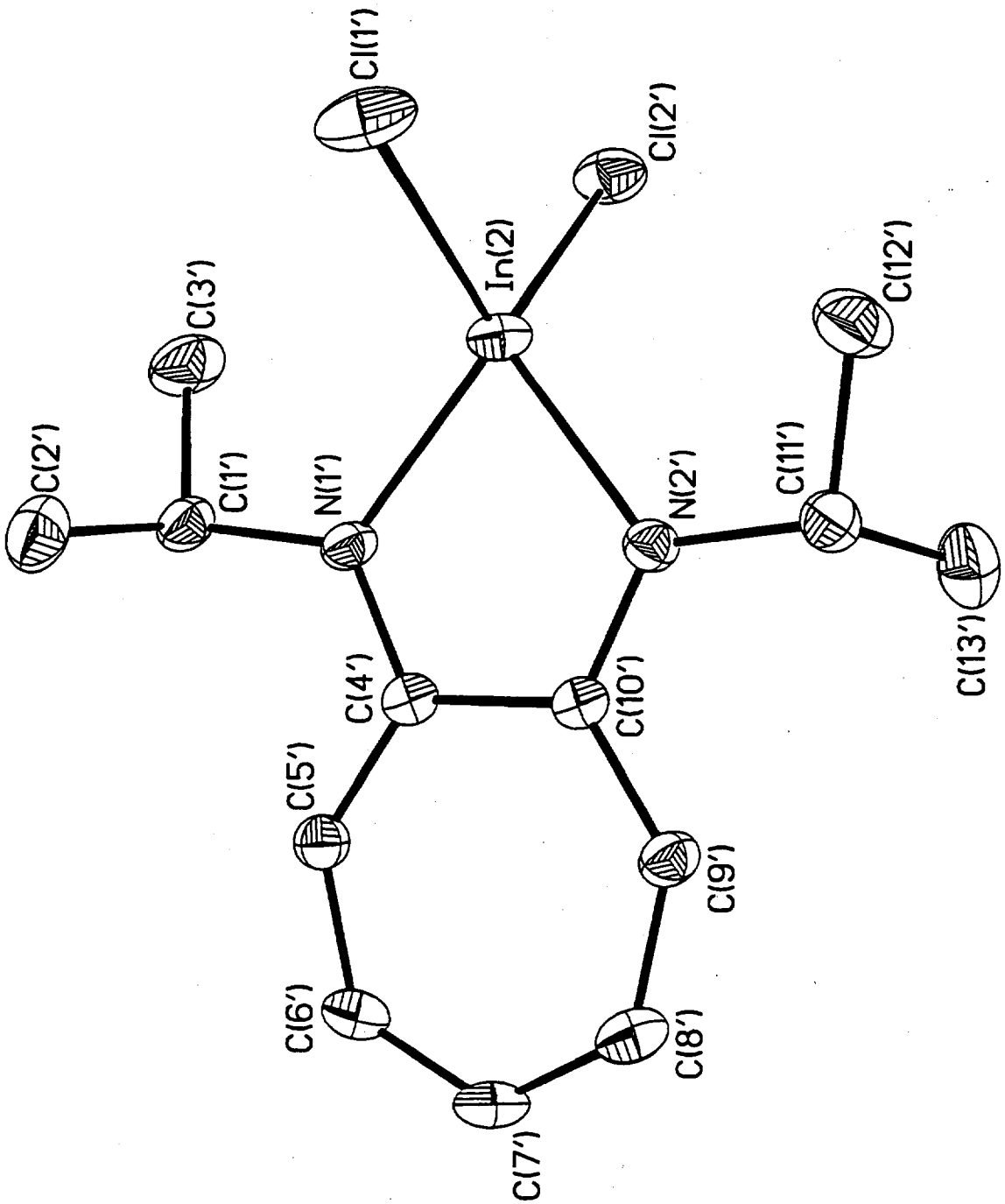
Cl(2)
In(1)
C(3)
C(12)
C(2)
N(1)
N(2)
C(13)
C(1)
C(11)
C(4)
C(10)
C(5)
C(9)
C(6)
C(8)
C(7)



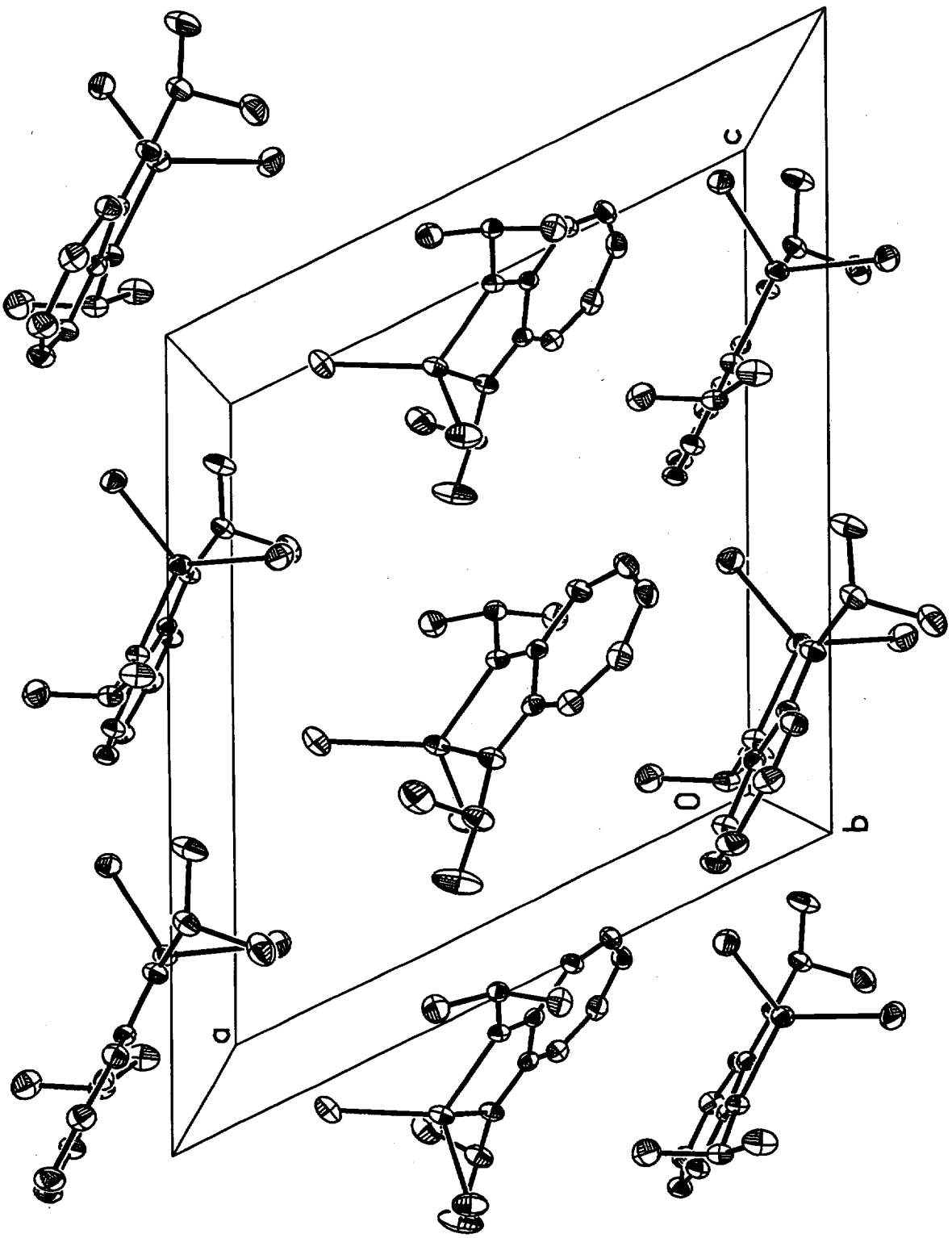

c
a
b
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Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
In(1)	4033(1)	3484(1)	1640(1)	34(1)
In(2)	9745(1)	3665(1)	2591(1)	34(1)
Cl(1)	4494(1)	2479(1)	2816(1)	58(1)
Cl(1')	11460(1)	3073(1)	3181(1)	60(1)
Cl(2')	8752(1)	2988(1)	1129(1)	49(1)
Cl(2)	2145(1)	3603(1)	845(1)	50(1)
N(1)	5004(2)	3463(1)	919(1)	30(1)
N(1')	9757(2)	4929(1)	2685(1)	33(1)
N(2)	4881(2)	4572(1)	2097(1)	34(1)
N(2')	9011(2)	3850(1)	3510(1)	32(1)
C(1)	4979(2)	2790(2)	284(2)	33(1)
C(1')	10289(2)	5441(2)	2243(2)	39(1)
C(2)	5973(2)	2254(2)	746(2)	46(1)
C(2')	11423(3)	5650(2)	2977(2)	56(1)
C(3')	10289(3)	4998(2)	1380(2)	59(1)
C(3)	3967(2)	2300(2)	47(2)	49(1)
C(4)	5612(2)	4126(1)	1035(2)	28(1)
C(4')	9328(2)	5232(2)	3243(2)	29(1)
C(5)	6276(2)	4198(2)	563(2)	36(1)
C(5')	9305(2)	6069(2)	3373(2)	36(1)
C(6)	6965(2)	4799(2)	545(2)	42(1)
C(6')	8866(2)	6552(2)	3843(2)	41(1)
C(7)	7204(2)	5541(2)	990(2)	42(1)
C(7')	8360(2)	6338(2)	4394(2)	43(1)
C(8)	6784(2)	5840(2)	1572(2)	41(1)
C(8')	8198(2)	5560(2)	4614(2)	43(1)
C(9)	6062(2)	5500(2)	1860(2)	36(1)
C(9')	8442(2)	4829(2)	4317(2)	36(1)
C(10)	5526(2)	4754(1)	1684(2)	30(1)
C(10')	8906(2)	4625(1)	3700(2)	28(1)
C(11)	4656(3)	5143(2)	2714(2)	45(1)

C(11')	8643(2)	3179(2)	3918(2)	37(1)
C(12)	4334(4)	4680(2)	3391(3)	86(1)
C(12')	9202(3)	2409(2)	3854(2)	54(1)
C(13)	3750(3)	5714(2)	2076(2)	63(1)
C(13')	7423(3)	3091(2)	3405(2)	56(1)

Table 2. Bond lengths [Å] and angles [°] for **3**.

In(1)-N(1)	2.093(2)
In(1)-N(2)	2.098(2)
In(1)-Cl(1)	2.3447(7)
In(1)-Cl(2)	2.3515(9)
In(2)-N(1')	2.103(2)
In(2)-N(2')	2.107(2)
In(2)-Cl(1')	2.3466(8)
In(2)-Cl(2')	2.3557(7)
N(1)-C(4)	1.346(3)
N(1)-C(1)	1.481(3)
N(1')-C(4')	1.344(3)
N(1')-C(1')	1.477(3)
N(2)-C(10)	1.342(3)
N(2)-C(11)	1.477(3)
N(2')-C(10')	1.342(3)
N(2')-C(11')	1.478(3)
C(1)-C(3)	1.516(4)
C(1)-C(2)	1.522(4)
C(1')-C(2')	1.515(4)
C(1')-C(3')	1.529(4)
C(4)-C(5)	1.411(3)
C(4)-C(10)	1.490(3)
C(4')-C(5')	1.406(3)
C(4')-C(10')	1.492(3)
C(5)-C(6)	1.388(4)
C(5')-C(6')	1.392(4)
C(6)-C(7)	1.380(4)
C(6')-C(7')	1.370(4)
C(7)-C(8)	1.366(4)
C(7')-C(8')	1.380(4)
C(8)-C(9)	1.381(4)
C(8')-C(9')	1.391(3)
C(9)-C(10)	1.408(3)
C(9')-C(10')	1.411(3)

C(11)-C(12)	1.519(4)
C(11)-C(13)	1.533(4)
C(11')-C(13')	1.520(4)
C(11')-C(12')	1.518(4)

N(1)-In(1)-N(2)	78.52(8)
N(1)-In(1)-Cl(1)	112.81(6)
N(2)-In(1)-Cl(1)	115.45(6)
N(1)-In(1)-Cl(2)	123.06(6)
N(2)-In(1)-Cl(2)	115.45(6)
Cl(1)-In(1)-Cl(2)	108.99(3)
N(1')-In(2)-N(2')	78.39(8)
N(1')-In(2)-Cl(1')	114.50(6)
N(2')-In(2)-Cl(1')	120.14(6)
N(1')-In(2)-Cl(2')	121.75(6)
N(2')-In(2)-Cl(2')	118.27(6)
Cl(1')-In(2)-Cl(2')	103.56(3)
C(4)-N(1)-C(1)	122.3(2)
C(4)-N(1)-In(1)	115.11(16)
C(1)-N(1)-In(1)	122.45(16)
C(4')-N(1')-C(1')	122.5(2)
C(4')-N(1')-In(2)	115.20(17)
C(1')-N(1')-In(2)	122.11(16)
C(10)-N(2)-C(11)	122.7(2)
C(10)-N(2)-In(1)	114.90(16)
C(11)-N(2)-In(1)	121.76(17)
C(10')-N(2')-C(11')	122.5(2)
C(10')-N(2')-In(2)	114.84(16)
C(11')-N(2')-In(2)	122.70(16)
N(1)-C(1)-C(3)	108.2(2)
N(1)-C(1)-C(2)	112.1(2)
C(3)-C(1)-C(2)	110.2(2)
N(1')-C(1')-C(2')	110.1(2)
N(1')-C(1')-C(3')	108.9(2)
C(2')-C(1')-C(3')	111.7(3)
N(1)-C(4)-C(5)	120.7(2)

N(1)-C(4)-C(10)	115.5(2)
C(5)-C(4)-C(10)	123.8(2)
N(1')-C(4')-C(5')	120.5(2)
N(1')-C(4')-C(10')	115.5(2)
C(5')-C(4')-C(10')	124.0(2)
C(6)-C(5)-C(4)	133.0(3)
C(6')-C(5')-C(4')	133.5(3)
C(7)-C(6)-C(5)	130.2(3)
C(7')-C(6')-C(5')	129.8(3)
C(8)-C(7)-C(6)	125.3(3)
C(6')-C(7')-C(8')	125.5(3)
C(7)-C(8)-C(9)	130.3(3)
C(7')-C(8')-C(9')	130.1(3)
C(8)-C(9)-C(10)	133.6(3)
C(8')-C(9')-C(10')	133.2(3)
N(2)-C(10)-C(9)	120.6(2)
N(2)-C(10)-C(4)	115.7(2)
C(9)-C(10)-C(4)	123.7(2)
N(2')-C(10')-C(9')	120.4(2)
N(2')-C(10')-C(4')	116.1(2)
C(9')-C(10')-C(4')	123.6(2)
N(2)-C(11)-C(12)	109.5(2)
N(2)-C(11)-C(13)	108.8(2)
C(12)-C(11)-C(13)	110.8(3)
N(2')-C(11')-C(13')	111.1(2)
N(2')-C(11')-C(12')	108.9(2)
C(13')-C(11')-C(12')	111.3(2)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
In(1)	47(1)	28(1)	37(1)	0(1)	27(1)	-2(1)
In(2)	40(1)	35(1)	31(1)	-1(1)	18(1)	9(1)
Cl(1)	90(1)	43(1)	51(1)	15(1)	41(1)	1(1)
Cl(1')	52(1)	79(1)	43(1)	0(1)	16(1)	32(1)
Cl(2')	48(1)	57(1)	40(1)	-14(1)	18(1)	6(1)
Cl(2)	46(1)	49(1)	68(1)	2(1)	38(1)	-2(1)
N(1)	36(1)	30(1)	25(1)	0(1)	15(1)	2(1)
N(1')	39(1)	34(1)	34(1)	2(1)	22(1)	5(1)
N(2)	45(2)	29(1)	35(1)	-3(1)	25(1)	-1(1)
N(2')	39(1)	30(1)	31(1)	1(1)	19(1)	1(1)
C(1)	35(2)	36(2)	29(1)	-5(1)	15(1)	1(1)
C(1')	42(2)	39(2)	45(2)	5(1)	28(1)	4(1)
C(2)	46(2)	38(2)	52(2)	-9(1)	20(2)	6(1)
C(2')	49(2)	57(2)	69(2)	12(2)	34(2)	1(2)
C(3')	80(3)	60(2)	59(2)	6(2)	53(2)	9(2)
C(3)	50(2)	48(2)	50(2)	-20(1)	24(2)	-7(2)
C(4)	31(2)	29(1)	23(1)	6(1)	10(1)	6(1)
C(4')	29(2)	33(1)	25(1)	2(1)	11(1)	4(1)
C(5)	40(2)	39(2)	36(1)	3(1)	22(1)	5(1)
C(5')	41(2)	33(1)	37(1)	2(1)	21(1)	1(1)
C(6)	36(2)	52(2)	43(2)	13(1)	24(1)	9(1)
C(6')	50(2)	31(2)	39(2)	-4(1)	18(1)	6(1)
C(7)	32(2)	44(2)	48(2)	15(1)	18(1)	-1(1)
C(7')	56(2)	40(2)	38(2)	-6(1)	24(1)	12(1)
C(8)	37(2)	35(2)	42(2)	7(1)	12(1)	-3(1)
C(8')	49(2)	51(2)	35(1)	-1(1)	25(1)	9(2)
C(9)	40(2)	32(1)	35(1)	1(1)	14(1)	2(1)
C(9')	43(2)	38(2)	34(1)	1(1)	23(1)	3(1)
C(10)	33(2)	27(1)	25(1)	6(1)	10(1)	6(1)
C(10')	26(2)	32(1)	23(1)	1(1)	9(1)	3(1)
C(11)	61(2)	37(2)	50(2)	-11(1)	37(2)	-5(2)

C(11')	49(2)	34(2)	32(1)	1(1)	21(1)	-2(1)
C(12)	158(4)	63(2)	80(3)	-17(2)	91(3)	-10(3)
C(12')	85(3)	34(2)	54(2)	2(1)	40(2)	3(2)
C(13)	73(3)	50(2)	78(2)	-15(2)	45(2)	3(2)
C(13')	56(2)	60(2)	49(2)	-1(2)	19(2)	-20(2)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3.

	x	y	z	U(eq)
H(1)	4946	3018	-324	40
H(1')	9867	5951	2014	46
H(2A)	6623	2582	925	69
H(2B)	5946	1838	289	69
H(2C)	5989	1999	1321	69
H(2'1)	11389	5977	3489	83
H(2'2)	11787	5955	2666	83
H(2'3)	11824	5153	3252	83
H(3'1)	10754	4522	1602	88
H(3'2)	10561	5358	1036	88
H(3'3)	9552	4830	949	88
H(3A)	4008	2050	634	73
H(3B)	3903	1880	-418	73
H(3C)	3336	2655	-227	73
H(5)	6245	3743	181	44
H(5')	9664	6367	3078	43
H(6)	7329	4680	165	50
H(6')	8927	7116	3772	49
H(7)	7702	5871	883	50
H(7')	8098	6762	4646	52
H(8)	7027	6364	1818	49
H(8')	7868	5516	5035	51
H(9)	5892	5844	2263	43
H(9')	8258	4374	4585	43
H(11)	5321	5465	3099	54
H(11')	8858	3297	4610	44
H(12A)	3680	4367	3016	129
H(12B)	4196	5059	3807	129
H(12C)	4920	4314	3785	129
H(12D)	9001	2287	3179	81

H(12E)	8979	1964	4141	81
H(12F)	9985	2480	4200	81
H(13A)	3962	5990	1628	94
H(13B)	3618	6112	2477	94
H(13C)	3090	5403	1713	94
H(13D)	7085	3602	3436	85
H(13E)	7196	2667	3715	85
H(13F)	7203	2947	2732	85

II. X-ray Crystallographic Analysis of (^{i}Pr$_2$-ATI)InMe$_2$ (**4**).

Crystallographic Experimental Section

Data Collection

A pale yellow air-sensitive crystal with approximate dimensions 0.46 x 0.25 x 0.15 mm^3 was selected under oil under ambient conditions and attached to the tip of a glass capillary. The crystal was mounted in a stream of cold nitrogen at 183(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 5.08 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° in a 6° range about ω with the exposure time of 10 seconds per frame. A total of 191 reflections was obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 6637 strong reflections from the actual data collection.

The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of 1.4 hemisphere to a resolution of 0.80 Å. A total of 44343 data were harvested by collecting two sets of frames with 0.3° scans in ω with an exposure time 10 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group *Pbca* that yielded chemically reasonable and computationally stable results of refinement [2]. A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen

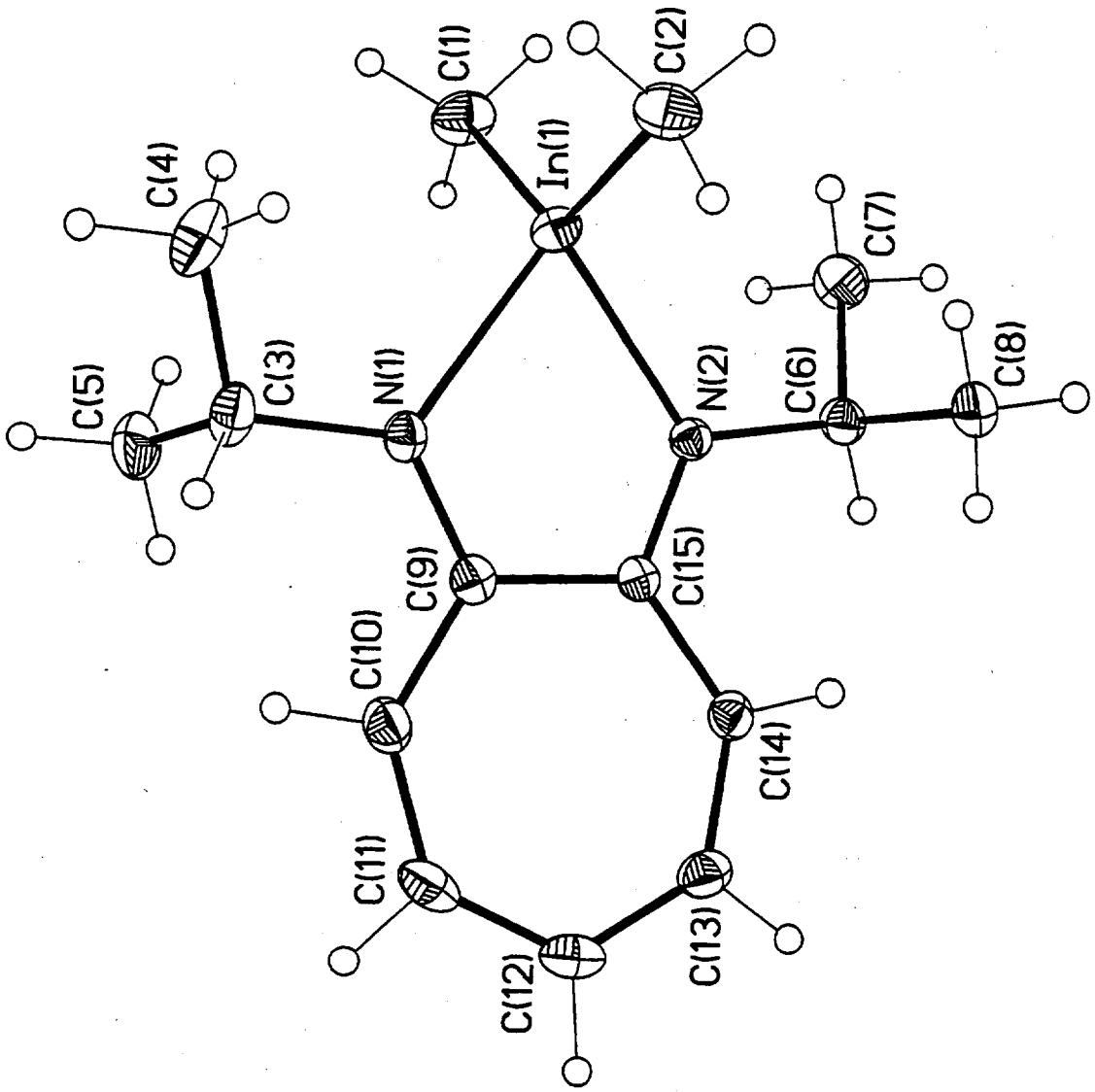
atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. There are two independent molecules of the complex in the asymmetric unit. The final least-squares refinement of 337 parameters against 6623 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0224 and 0.0436, respectively. The final difference Fourier map was featureless.

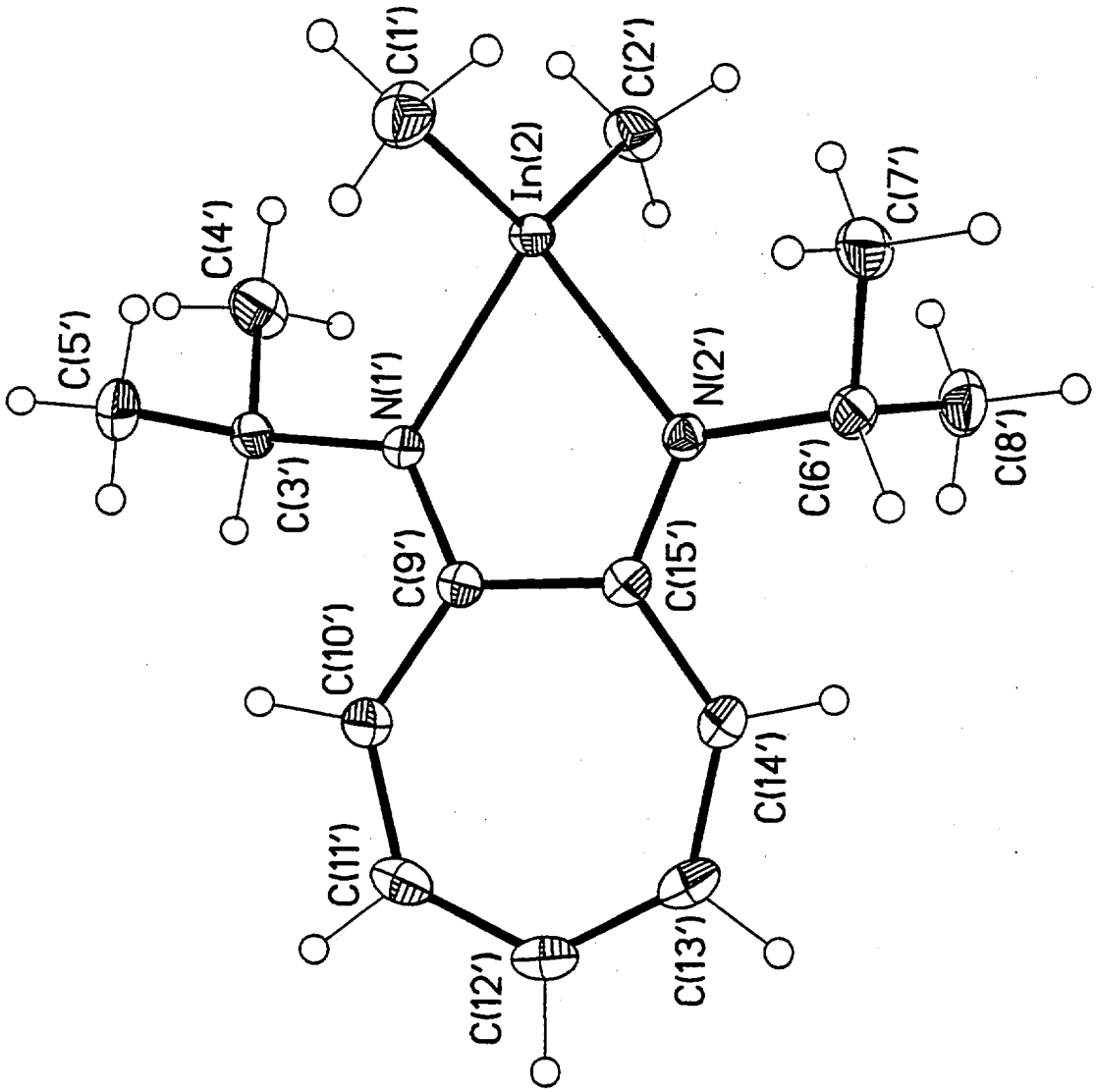
References

[1] Blessing, R.H. *Acta Cryst.* **1995**, *A51*, 33-38.

[2] All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).

Crystal data and structure refinement for **4**		
Identification code	jor18	
Empirical formula	$C_{15}H_{25}InN_2$	
Formula weight	348.19	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 20.7956(11) Å	α= 90°
	b = 9.2365(5) Å	β= 90°
	c = 33.7109(18) Å	γ = 90°
Volume	6475.1(6) $Å^3$	
Z	16	
Density (calculated)	1.429 Mg/m^3	
Absorption coefficient	1.447 mm^{-1}	
F(000)	2848	
Crystal size	0.46 x 0.25 x 0.15 mm^3	
Theta range for data collection	1.21 to 26.37°.	
Index ranges	0<=h<=25, 0<=k<=11, 0<=l<=42	
Reflections collected	44343	
Independent reflections	6623 [R(int) = 0.0372]	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.8122 and 0.5557	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6623 / 0 / 337	
Goodness-of-fit on F^2	1.021	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0436	
R indices (all data)	R1 = 0.0414, wR2 = 0.0470	
Largest diff. peak and hole	0.305 and -0.302 $e.Å^{-3}$	

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C(2')
In(2)
C(4')
C(7')
C(5')
N(1')
N(2')
C(3')
C(6')
C(8')
C(9')
C(15')
C(10')
C(14')
C(11')
C(13')
C(12')

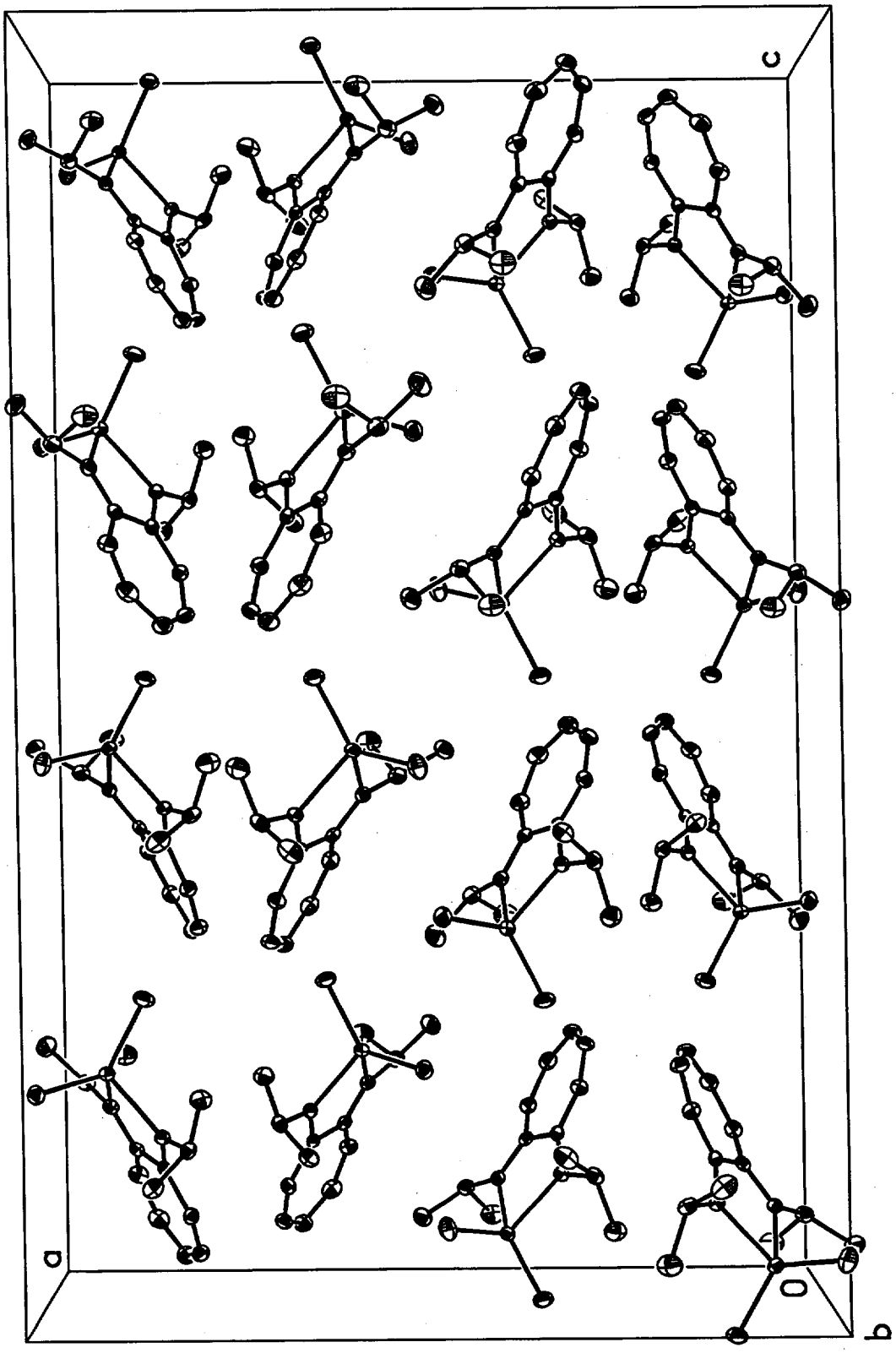

c
a
O
b

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
In(1)	4059(1)	7012(1)	-1950(1)	28(1)
N(1)	4109(1)	9029(2)	-1612(1)	27(1)
N(2)	3376(1)	6782(2)	-1461(1)	24(1)
C(1)	3600(1)	7411(3)	-2515(1)	44(1)
C(2)	4870(1)	5623(3)	-1836(1)	40(1)
C(3)	4482(1)	10263(3)	-1764(1)	37(1)
C(4)	4959(1)	9749(3)	-2071(1)	53(1)
C(5)	4028(1)	11373(3)	-1949(1)	52(1)
C(6)	3004(1)	5436(2)	-1415(1)	29(1)
C(7)	2823(1)	4850(3)	-1823(1)	44(1)
C(8)	3396(1)	4323(2)	-1184(1)	38(1)
C(9)	3791(1)	9083(2)	-1271(1)	25(1)
C(10)	3828(1)	10317(3)	-1018(1)	35(1)
C(11)	3587(1)	10626(3)	-648(1)	41(1)
C(12)	3204(1)	9812(3)	-398(1)	40(1)
C(13)	2974(1)	8444(3)	-483(1)	34(1)
C(14)	3058(1)	7589(2)	-814(1)	29(1)
C(15)	3394(1)	7781(2)	-1176(1)	22(1)
In(2)	4088(1)	5311(1)	555(1)	25(1)
N(1')	3388(1)	5523(2)	1035(1)	24(1)
N(2')	4182(1)	3340(2)	908(1)	24(1)
C(1')	4861(1)	6809(3)	670(1)	46(1)
C(2')	3633(1)	4767(3)	0(1)	41(1)
C(3')	2993(1)	6833(2)	1077(1)	32(1)
C(4')	2755(1)	7305(3)	669(1)	53(1)
C(5')	3372(1)	8043(2)	1272(1)	48(1)
C(6')	4604(1)	2150(2)	781(1)	32(1)
C(7')	5184(1)	2785(3)	570(1)	43(1)
C(8')	4245(1)	1103(3)	507(1)	48(1)
C(9')	3418(1)	4538(2)	1322(1)	23(1)
C(10')	3128(1)	4771(3)	1698(1)	32(1)

C(11')	3024(1)	3883(3)	2021(1)	37(1)
C(12')	3158(1)	2441(3)	2074(1)	38(1)
C(13')	3471(1)	1567(3)	1803(1)	37(1)
C(14')	3749(1)	1913(2)	1441(1)	30(1)
C(15')	3803(1)	3224(2)	1225(1)	25(1)

Table 2. Bond lengths [Å] and angles [°] for **4**.

In(1)-C(2)	2.153(2)
In(1)-C(1)	2.161(2)
In(1)-N(2)	2.1868(17)
In(1)-N(1)	2.1871(18)
N(1)-C(9)	1.328(3)
N(1)-C(3)	1.470(3)
N(2)-C(15)	1.334(3)
N(2)-C(6)	1.472(3)
C(3)-C(4)	1.512(3)
C(3)-C(5)	1.525(3)
C(6)-C(8)	1.525(3)
C(6)-C(7)	1.526(3)
C(9)-C(10)	1.426(3)
C(9)-C(15)	1.494(3)
C(10)-C(11)	1.375(3)
C(11)-C(12)	1.380(3)
C(12)-C(13)	1.381(3)
C(13)-C(14)	1.377(3)
C(14)-C(15)	1.418(3)
In(2)-C(1')	2.156(2)
In(2)-C(2')	2.157(2)
In(2)-N(2')	2.1838(17)
In(2)-N(1')	2.1839(17)
N(1')-C(9')	1.331(3)
N(1')-C(3')	1.470(3)
N(2')-C(15')	1.332(3)
N(2')-C(6')	1.470(3)
C(3')-C(5')	1.518(3)
C(3')-C(4')	1.526(3)
C(6')-C(7')	1.518(3)
C(6')-C(8')	1.531(3)
C(9')-C(10')	1.420(3)
C(9')-C(15')	1.492(3)
C(10')-C(11')	1.380(3)

C(11')-C(12')	1.373(3)
C(12')-C(13')	1.383(3)
C(13')-C(14')	1.386(3)
C(14')-C(15')	1.418(3)

C(2)-In(1)-C(1)	127.23(10)
C(2)-In(1)-N(2)	108.43(8)
C(1)-In(1)-N(2)	113.15(9)
C(2)-In(1)-N(1)	112.16(8)
C(1)-In(1)-N(1)	109.59(9)
N(2)-In(1)-N(1)	73.78(6)
C(9)-N(1)-C(3)	122.35(19)
C(9)-N(1)-In(1)	117.38(14)
C(3)-N(1)-In(1)	120.27(14)
C(15)-N(2)-C(6)	121.43(18)
C(15)-N(2)-In(1)	117.27(14)
C(6)-N(2)-In(1)	120.25(13)
N(1)-C(3)-C(4)	109.9(2)
N(1)-C(3)-C(5)	109.7(2)
C(4)-C(3)-C(5)	109.7(2)
N(2)-C(6)-C(8)	110.13(19)
N(2)-C(6)-C(7)	109.41(18)
C(8)-C(6)-C(7)	110.69(19)
N(1)-C(9)-C(10)	121.4(2)
N(1)-C(9)-C(15)	115.54(19)
C(10)-C(9)-C(15)	123.1(2)
C(11)-C(10)-C(9)	133.6(2)
C(10)-C(11)-C(12)	130.5(2)
C(11)-C(12)-C(13)	125.0(2)
C(14)-C(13)-C(12)	130.3(2)
C(13)-C(14)-C(15)	133.5(2)
N(2)-C(15)-C(14)	121.4(2)
N(2)-C(15)-C(9)	114.69(19)
C(14)-C(15)-C(9)	123.9(2)
C(1')-In(2)-C(2')	129.22(10)
C(1')-In(2)-N(2')	111.70(8)

C(2')-In(2)-N(2')	108.58(8)
C(1')-In(2)-N(1')	107.84(8)
C(2')-In(2)-N(1')	111.78(9)
N(2')-In(2)-N(1')	74.42(6)
C(9')-N(1')-C(3')	121.19(18)
C(9')-N(1')-In(2)	116.56(14)
C(3')-N(1')-In(2)	121.20(13)
C(15')-N(2')-C(6')	121.77(18)
C(15')-N(2')-In(2)	116.81(14)
C(6')-N(2')-In(2)	121.21(13)
N(1')-C(3')-C(5')	111.0(2)
N(1')-C(3')-C(4')	109.17(18)
C(5')-C(3')-C(4')	110.5(2)
N(2')-C(6')-C(7')	108.74(18)
N(2')-C(6')-C(8')	111.0(2)
C(7')-C(6')-C(8')	110.4(2)
N(1')-C(9')-C(10')	121.8(2)
N(1')-C(9')-C(15')	114.88(19)
C(10')-C(9')-C(15')	123.2(2)
C(11')-C(10')-C(9')	132.9(2)
C(12')-C(11')-C(10')	130.3(2)
C(11')-C(12')-C(13')	125.2(2)
C(12')-C(13')-C(14')	130.1(2)
C(13')-C(14')-C(15')	133.0(2)
N(2')-C(15')-C(14')	121.9(2)
N(2')-C(15')-C(9')	115.41(18)
C(14')-C(15')-C(9')	122.6(2)

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
In(1)	28(1)	33(1)	22(1)	-1(1)	1(1)	0(1)
N(1)	27(1)	26(1)	28(1)	3(1)	-4(1)	-5(1)
N(2)	25(1)	23(1)	24(1)	0(1)	0(1)	-2(1)
C(1)	50(2)	56(2)	26(1)	1(1)	-8(1)	5(1)
C(2)	34(2)	44(2)	42(2)	-7(1)	0(1)	5(1)
C(3)	40(2)	37(2)	34(1)	9(1)	-4(1)	-14(1)
C(4)	45(2)	59(2)	54(2)	19(1)	10(1)	-12(2)
C(5)	71(2)	33(2)	52(2)	14(1)	1(2)	-2(2)
C(6)	28(1)	26(1)	34(1)	-3(1)	4(1)	-6(1)
C(7)	50(2)	40(2)	41(2)	-7(1)	-3(1)	-17(1)
C(8)	45(2)	27(2)	42(2)	3(1)	8(1)	-2(1)
C(9)	24(1)	26(1)	26(1)	3(1)	-6(1)	3(1)
C(10)	42(2)	29(1)	35(2)	0(1)	-4(1)	-5(1)
C(11)	52(2)	30(2)	41(2)	-13(1)	-9(1)	3(1)
C(12)	43(2)	46(2)	31(1)	-12(1)	2(1)	8(1)
C(13)	35(2)	39(2)	28(1)	1(1)	6(1)	6(1)
C(14)	28(1)	27(1)	31(1)	2(1)	2(1)	2(1)
C(15)	20(1)	22(1)	25(1)	2(1)	-2(1)	4(1)
In(2)	26(1)	25(1)	24(1)	2(1)	3(1)	1(1)
N(1')	25(1)	22(1)	24(1)	0(1)	2(1)	1(1)
N(2')	25(1)	23(1)	24(1)	1(1)	-2(1)	3(1)
C(1')	36(2)	38(2)	65(2)	-1(1)	8(1)	-5(1)
C(2')	47(2)	49(2)	28(1)	0(1)	-4(1)	8(1)
C(3')	38(2)	27(1)	32(1)	1(1)	10(1)	10(1)
C(4')	61(2)	53(2)	45(2)	7(1)	4(2)	32(2)
C(5')	63(2)	26(2)	56(2)	-6(1)	17(2)	5(1)
C(6')	37(2)	30(1)	30(1)	4(1)	-1(1)	10(1)
C(7')	40(2)	44(2)	44(2)	7(1)	8(1)	17(1)
C(8')	68(2)	32(2)	45(2)	-9(1)	1(1)	7(1)
C(9')	21(1)	25(1)	24(1)	-2(1)	-3(1)	-5(1)
C(10')	34(2)	32(1)	30(1)	0(1)	2(1)	-1(1)

C(11')	39(2)	50(2)	24(1)	-1(1)	4(1)	-6(1)
C(12')	39(2)	47(2)	28(1)	12(1)	0(1)	-9(1)
C(13')	38(2)	33(2)	39(1)	13(1)	-8(1)	-10(1)
C(14')	32(2)	26(1)	33(1)	2(1)	-4(1)	-1(1)
C(15')	23(1)	26(1)	25(1)	0(1)	-7(1)	-4(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	3894	7954	-2687	66
H(1B)	3207	7974	-2474	66
H(1C)	3492	6485	-2641	66
H(2A)	4771	4639	-1926	60
H(2B)	4961	5611	-1551	60
H(2C)	5247	5987	-1979	60
H(3)	4719	10726	-1539	44
H(4A)	5219	8963	-1960	79
H(4B)	5240	10554	-2147	79
H(4C)	4728	9397	-2305	79
H(5A)	3806	10936	-2175	78
H(5B)	4276	12214	-2038	78
H(5C)	3711	11681	-1751	78
H(6)	2602	5654	-1264	35
H(7A)	2599	5603	-1974	65
H(7B)	2541	4008	-1792	65
H(7C)	3214	4561	-1965	65
H(8A)	3795	4112	-1327	57
H(8B)	3145	3431	-1154	57
H(8C)	3500	4710	-921	57
H(10)	4071	11089	-1128	42
H(11)	3702	11551	-547	49
H(12)	3091	10224	-150	48
H(13)	2716	8025	-280	41
H(14)	2846	6680	-795	34
H(1'1)	5263	6416	564	70
H(1'2)	4904	6954	957	70
H(1'3)	4766	7737	542	70
H(2'1)	3511	5658	-139	62
H(2'2)	3247	4186	51	62

H(2'3)	3933	4211	-165	62
H(3')	2612	6601	1247	39
H(4'1)	3123	7576	503	80
H(4'2)	2467	8138	697	80
H(4'3)	2522	6504	543	80
H(5'1)	3509	7736	1538	72
H(5'2)	3101	8907	1294	72
H(5'3)	3752	8267	1111	72
H(6')	4754	1609	1021	39
H(7'1)	5042	3311	333	64
H(7'2)	5476	2003	492	64
H(7'3)	5408	3451	749	64
H(8'1)	3868	715	645	72
H(8'2)	4531	304	433	72
H(8'3)	4106	1617	268	72
H(10')	2974	5731	1735	38
H(11')	2828	4344	2242	45
H(12')	3026	2009	2317	46
H(13')	3499	575	1875	44
H(14')	3943	1109	1313	36

[{1,2-(N^{i}Pr)$_2$-5-CPh$_3$-cyclohepta-3,6-diene}InMe$_2$][B(C$_6$F$_5$)$_4$] (**5**).

Crystallographic Experimental Section

Data Collection

A yellow crystal with approximate dimensions 0.40 x 0.30 x 0.30 mm^3 was selected under oil under ambient conditions and attached to the tip of a glass capillary. The crystal was mounted in a stream of cold nitrogen at 183(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α (λ = 0.71073 Å) radiation and the diffractometer to crystal distance of 5.08 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° in a 6° range about ω with the exposure time of 10 seconds per frame. A total of 172 reflections was obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 8192 strong reflections from the actual data collection.

The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of 1.2 hemisphere to a resolution of 0.80 Å. A total of 14924 data were harvested by collecting two sets of frames with 0.4° scans in ω with an exposure time 10 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were consistent for the space groups $P1$ and $P\bar{1}$ [2]. The *E*-statistics strongly suggested the centrosymmetric space group $P\bar{1}$ that yielded chemically reasonable and computationally stable results of refinement. A successful solution by the direct methods provided most non-hydrogen atoms from the *E*-map. The remaining non-hydrogen atoms were located in an

alternating series of least squares cycles and difference Fourier maps. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients. The final least-squares refinement of 745 parameters against 9641 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0280 and 0.0729, respectively. The final difference Fourier map was featureless.

The ORTEP diagrams were drawn with 30% probability ellipsoids.

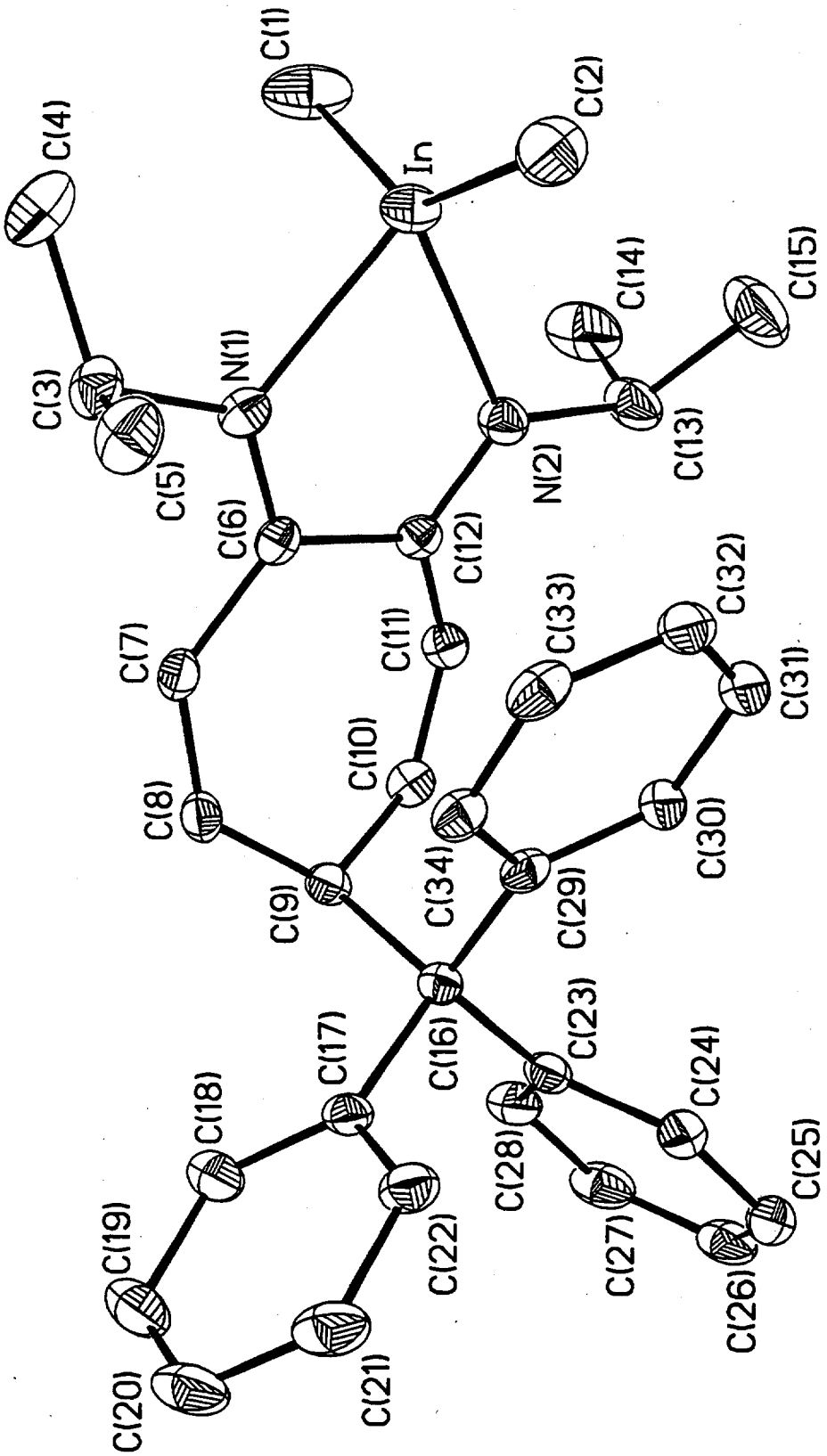
References

[1] Blessing, R.H. *Acta Cryst.* **1995**, *A51*, 33-38.

[2] All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).

Crystal data and structure refinement for **5**

Identification code	jor20	
Empirical formula	$C_{58}\ H_{40}\ B\ F_{20}\ In\ N_2$	
Formula weight	1270.55	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.3595(6) Å	α= 89.939(1)°
	b = 14.2584(7) Å	β= 88.532(1)°
	c = 17.0182(8) Å	γ = 70.431(1)°
Volume	2596.3(2) $Å^3$	
Z	2	
Density (calculated)	1.625 Mg/m^3	
Absorption coefficient	0.570 mm^{-1}	
F(000)	1272	
Crystal size	0.40 x 0.35 x 0.35 mm^3	
Theta range for data collection	1.52 to 26.37°.	
Index ranges	-13<=h<=14, -17<=k<=17, 0<=l<=21	
Reflections collected	14924	
Independent reflections	9641 [R(int) = 0.0119]	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.8255 and 0.8041	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9641 / 0 / 745	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0280, wR2 = 0.0729	
R indices (all data)	R1 = 0.0358, wR2 = 0.0765	
Largest diff. peak and hole	0.393 and -0.356 $e.Å^{-3}$	


C(1)
C(2)
C(4)
In
C(14)
C(15)
C(3)
N(1)
C(13)
C(5)
N(2)
C(6)
C(12)
C(32)
C(7)
C(11)
C(33)
C(31)
C(10)
C(8)
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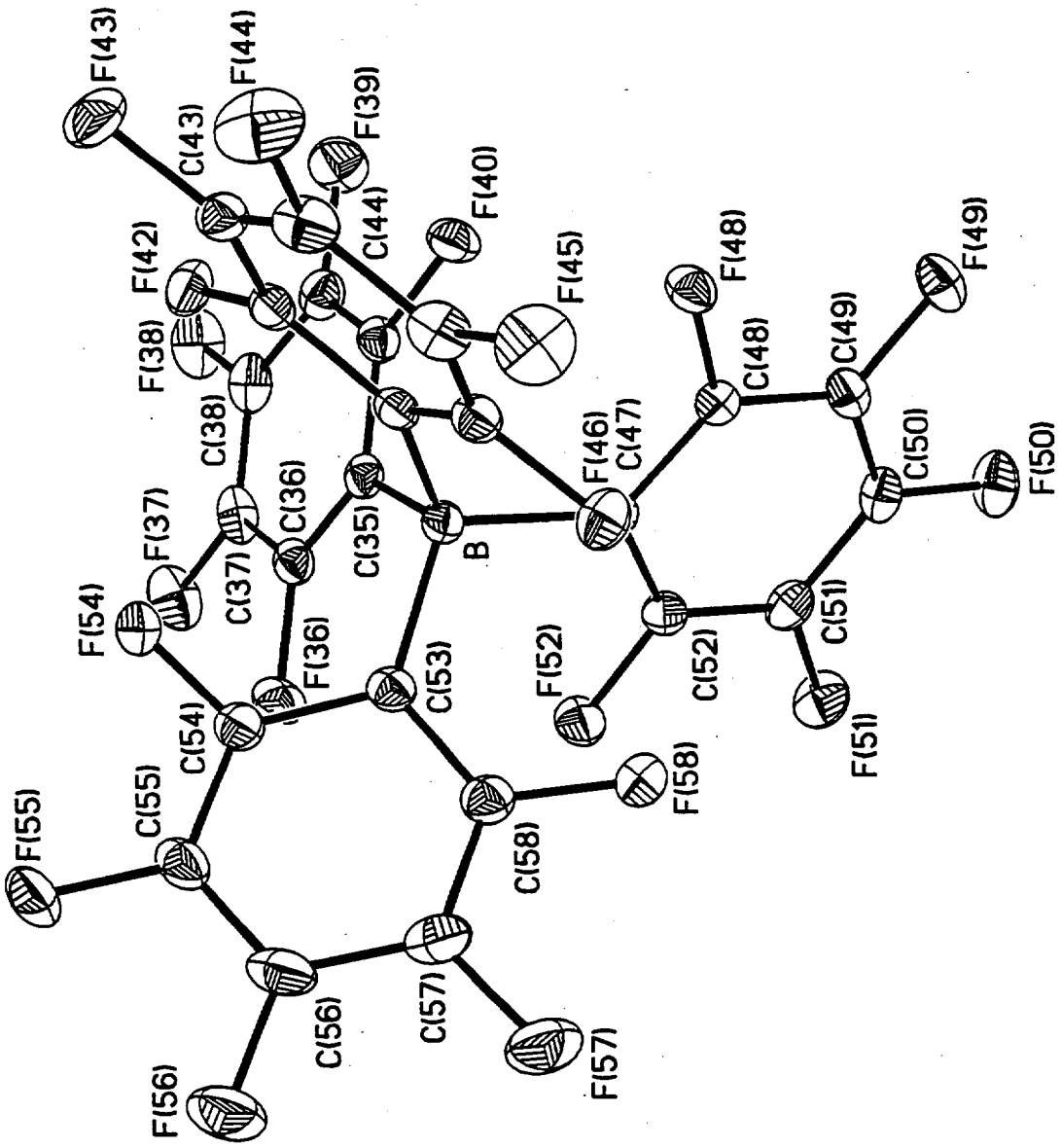
F(43)
F(44)
C(43)
F(39)
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F(40)
F(42)
F(45)
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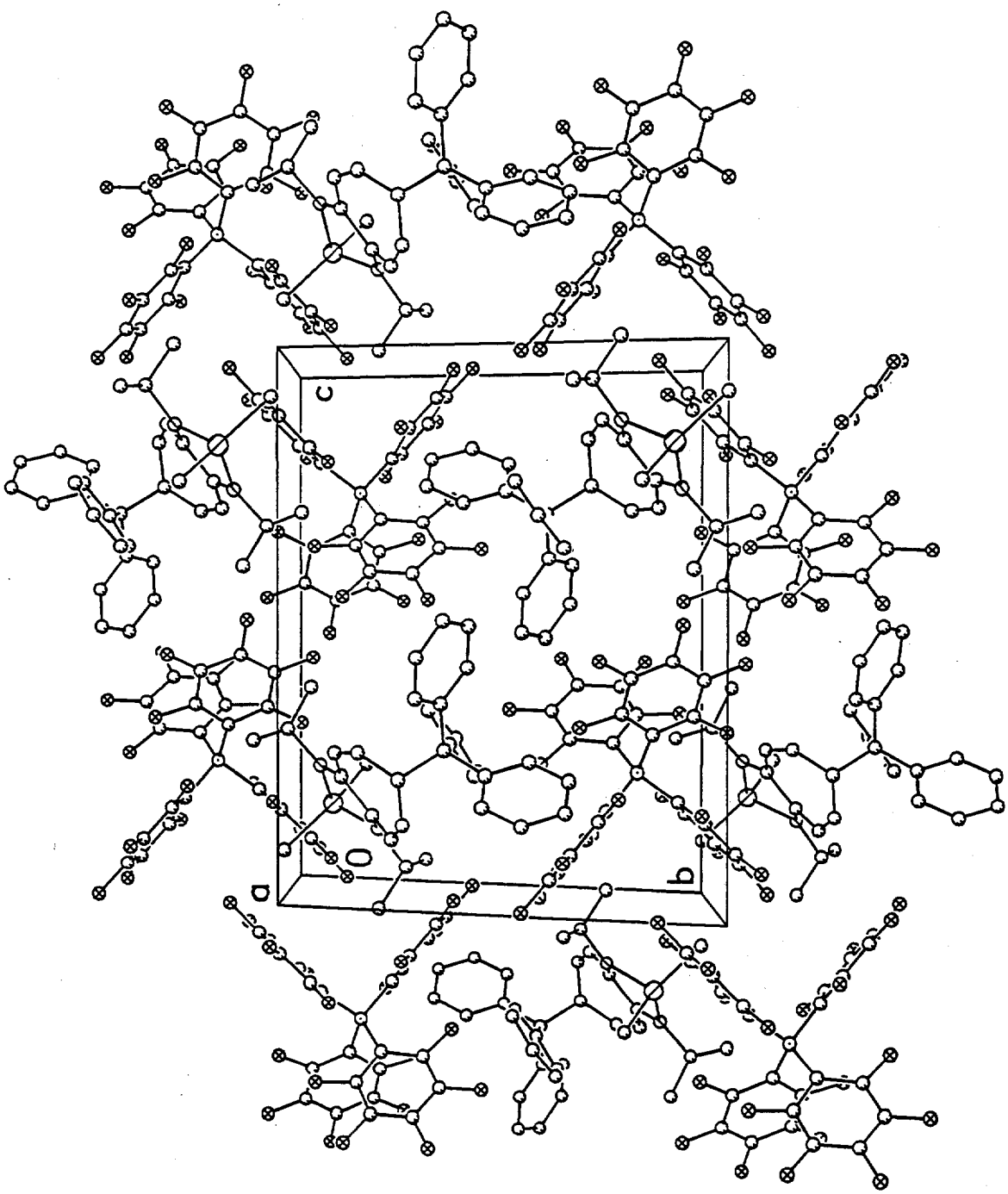

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5.** U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
In	8073(1)	1220(1)	1806(1)	36(1)
F(36)	8274(1)	-2269(1)	2040(1)	41(1)
F(37)	9531(1)	-3530(1)	928(1)	55(1)
F(38)	8369(1)	-4431(1)	-36(1)	58(1)
F(39)	5834(1)	-3990(1)	118(1)	54(1)
F(40)	4549(1)	-2757(1)	1244(1)	39(1)
F(42)	5598(1)	-3953(1)	2546(1)	40(1)
F(43)	4286(1)	-4668(1)	3516(1)	50(1)
F(44)	2445(2)	-3431(1)	4473(1)	61(1)
F(45)	2017(1)	-1437(1)	4432(1)	55(1)
F(46)	3386(1)	-698(1)	3490(1)	39(1)
F(48)	2667(1)	-1065(1)	1941(1)	34(1)
F(49)	1680(1)	306(1)	889(1)	41(1)
F(50)	3044(1)	1344(1)	182(1)	47(1)
F(51)	5414(1)	1046(1)	661(1)	50(1)
F(52)	6446(1)	-346(1)	1724(1)	43(1)
F(54)	7509(1)	-3118(1)	3272(1)	40(1)
F(55)	8750(2)	-2712(1)	4468(1)	63(1)
F(56)	8022(2)	-853(1)	5109(1)	72(1)
F(57)	6133(2)	639(1)	4445(1)	65(1)
F(58)	5017(1)	295(1)	3190(1)	44(1)
N(1)	9768(2)	992(1)	2537(1)	31(1)
N(2)	9014(2)	2311(1)	1402(1)	34(1)
B	5436(2)	-1748(2)	2437(1)	27(1)
C(1)	8701(3)	70(2)	942(2)	64(1)
C(2)	6429(2)	1965(2)	2491(2)	55(1)
C(3)	10024(2)	244(2)	3179(1)	40(1)
C(4)	9557(3)	-598(2)	2944(2)	58(1)
C(5)	9390(3)	756(2)	3926(1)	52(1)
C(6)	10474(2)	1513(1)	2377(1)	27(1)
C(7)	11601(2)	1406(1)	2816(1)	31(1)