

C(12A)	41(6)	40(7)	28(5)	-11(5)	2(5)	3(5)
C(13A)	34(6)	67(8)	39(6)	3(6)	10(5)	-13(6)
C(14A)	140(20)	73(17)	75(17)	18(13)	30(14)	33(15)
In(3)	39(1)	29(1)	36(1)	-1(1)	-3(1)	4(1)
N(1B)	22(4)	18(5)	24(5)	-3(4)	-4(4)	-2(4)
N(2B)	28(4)	46(6)	20(4)	5(4)	6(4)	8(4)
C(1B)	72(10)	15(6)	71(9)	5(6)	-14(8)	-7(6)
C(2B)	46(7)	41(7)	26(6)	0(5)	-5(5)	-4(5)
C(3B)	44(9)	75(16)	40(13)	10(14)	-5(7)	-14(11)
C(4B)	41(8)	43(8)	31(8)	4(6)	-3(7)	-7(8)
C(5B)	23(5)	37(6)	34(6)	15(5)	5(4)	1(5)
C(6B)	51(7)	28(6)	53(7)	13(5)	2(5)	17(5)
C(8B)	115(13)	49(9)	44(9)	18(8)	-25(9)	-16(9)
C(9B)	80(9)	60(9)	49(8)	22(7)	-20(7)	23(7)
C(10B)	78(9)	48(8)	25(6)	2(6)	-12(6)	24(7)
C(11B)	34(8)	40(8)	28(7)	2(6)	18(6)	-8(6)
C(12B)	36(6)	56(8)	25(6)	3(5)	2(5)	-9(5)
C(13B)	20(6)	67(13)	19(7)	-29(8)	9(6)	-22(7)
C(14B)	80(9)	59(9)	28(6)	-13(6)	1(6)	5(7)
Cl(1)	92(3)	49(2)	57(2)	-14(2)	-10(2)	-8(2)
C(100)	72(8)	33(7)	57(8)	-17(6)	2(7)	-11(6)
C(101)	99(11)	46(8)	45(8)	-3(6)	20(8)	-2(7)
C(102)	102(12)	57(10)	49(8)	-5(7)	2(9)	23(9)
C(103)	137(16)	67(11)	41(9)	11(8)	-11(10)	28(10)
Cl(2)	50(2)	70(2)	82(3)	18(2)	-8(2)	-19(2)
C(200)	19(5)	95(10)	40(7)	5(7)	-3(5)	-7(6)
C(201)	34(7)	98(11)	50(8)	-11(7)	-1(6)	-5(7)
C(202)	34(7)	142(16)	55(9)	20(10)	18(7)	30(9)
C(203)	67(10)	79(13)	57(10)	-6(9)	-6(8)	17(9)
C(204)	75(10)	67(11)	94(12)	-24(10)	26(9)	-8(9)
C(205)	86(12)	38(9)	46(9)	-1(7)	24(9)	-15(8)
Cl(3)	60(2)	56(2)	116(3)	-11(2)	15(2)	5(2)
C(300)	30(6)	51(7)	53(7)	-13(6)	2(5)	-12(5)
C(301)	75(9)	91(12)	45(8)	-23(8)	27(7)	-44(9)
C(302)	82(10)	72(10)	62(9)	12(8)	-11(7)	-39(8)
C(303)	64(8)	41(8)	90(10)	1(8)	-22(8)	-24(6)

C(304)	61(10)	60(10)	44(8)	-13(7)	-10(8)	-9(8)
C(305)	36(6)	50(7)	36(6)	1(6)	-6(5)	-11(5)
Cl(4)	55(2)	58(3)	124(4)	-18(2)	-15(2)	10(2)
C(400)	45(7)	28(6)	66(8)	-8(6)	8(6)	-6(5)
C(401)	53(7)	36(7)	63(8)	-8(6)	-6(6)	-3(6)
C(402)	59(8)	51(9)	55(9)	-23(7)	13(7)	-2(7)
C(403)	49(8)	58(9)	107(12)	-27(8)	-18(8)	-3(7)
C(404)	110(12)	50(9)	60(9)	4(7)	-8(8)	-14(9)
C(405)	63(8)	57(9)	56(8)	-1(7)	31(7)	4(7)
B(2)	34(3)	24(3)	25(3)	-2(2)	-6(2)	1(3)
F(16A)	45(2)	47(2)	34(2)	14(1)	-4(1)	-6(1)
F(17A)	69(2)	40(2)	47(2)	10(2)	10(2)	-11(2)
F(18A)	47(2)	46(2)	73(2)	-6(2)	9(2)	-21(2)
F(19A)	42(2)	56(2)	71(2)	1(2)	-20(2)	-15(2)
F(20A)	42(2)	38(2)	48(2)	6(1)	-20(1)	-4(1)
F(22A)	56(2)	29(2)	38(2)	-9(1)	2(1)	-7(1)
F(23A)	70(2)	41(2)	27(2)	-9(1)	4(1)	10(2)
F(24A)	38(2)	61(2)	36(2)	10(2)	9(1)	10(2)
F(25A)	44(2)	43(2)	56(2)	7(2)	5(1)	-12(2)
F(26A)	46(2)	32(2)	40(2)	-8(1)	3(1)	-9(1)
F(28A)	46(2)	57(2)	38(2)	2(2)	7(1)	2(2)
F(29A)	65(2)	82(3)	78(2)	-9(2)	41(2)	2(2)
F(30A)	54(2)	49(2)	138(3)	-3(2)	44(2)	14(2)
F(31A)	56(2)	50(2)	101(3)	16(2)	5(2)	21(2)
F(32A)	51(2)	40(2)	45(2)	6(2)	-4(2)	12(1)
F(34A)	41(2)	51(2)	45(2)	-17(2)	-5(1)	-7(2)
F(35A)	51(2)	95(3)	45(2)	-13(2)	-16(2)	-20(2)
F(36A)	32(2)	108(3)	63(2)	24(2)	-14(2)	-1(2)
F(37A)	41(2)	61(2)	73(2)	19(2)	5(2)	17(2)
F(38A)	45(2)	32(2)	45(2)	0(1)	0(1)	6(1)
C(15A)	30(3)	26(3)	27(3)	-4(2)	3(2)	-2(2)
C(16A)	29(3)	36(3)	27(3)	-6(2)	1(2)	2(2)
C(17A)	50(3)	28(3)	34(3)	5(2)	11(3)	-1(3)
C(18A)	33(3)	33(3)	46(3)	-8(3)	8(3)	-8(2)
C(19A)	34(3)	42(3)	38(3)	-9(3)	-10(2)	-4(2)
C(20A)	31(3)	25(3)	36(3)	0(2)	-3(2)	-1(2)

C(21A)	26(2)	23(3)	30(3)	2(2)	-6(2)	2(2)
C(22A)	33(3)	23(3)	31(3)	0(2)	-3(2)	-2(2)
C(23A)	38(3)	25(3)	29(3)	-4(2)	-8(2)	9(2)
C(24A)	27(3)	41(3)	27(3)	7(2)	-1(2)	14(2)
C(25A)	28(3)	25(3)	39(3)	5(2)	-5(2)	-2(2)
C(26A)	33(3)	24(3)	26(3)	-1(2)	-1(2)	2(2)
C(27A)	27(3)	26(3)	37(3)	-10(2)	-6(2)	-6(2)
C(28A)	27(3)	40(3)	39(3)	-5(3)	4(2)	-2(2)
C(29A)	42(3)	51(4)	58(4)	-15(3)	30(3)	-12(3)
C(30A)	33(3)	33(3)	86(5)	-9(3)	21(3)	6(2)
C(31A)	36(3)	26(3)	78(4)	5(3)	1(3)	3(2)
C(32A)	36(3)	27(3)	44(3)	-7(3)	-1(2)	-6(2)
C(33A)	24(2)	35(3)	27(3)	7(2)	2(2)	-4(2)
C(34A)	33(3)	38(3)	28(3)	-3(2)	1(2)	0(2)
C(35A)	34(3)	67(4)	26(3)	-4(3)	-5(2)	-15(3)
C(36A)	26(3)	74(4)	37(3)	16(3)	-5(2)	-4(3)
C(37A)	33(3)	42(3)	44(3)	12(3)	6(3)	4(3)
C(38A)	28(3)	34(3)	27(3)	4(2)	-2(2)	-5(2)
B(1)	27(3)	19(3)	28(3)	3(2)	-9(2)	2(2)
F(16)	41(2)	30(2)	38(2)	-6(1)	-3(1)	-8(1)
F(17)	46(2)	42(2)	48(2)	6(2)	0(1)	-18(1)
F(18)	38(2)	55(2)	40(2)	8(2)	10(1)	2(1)
F(19)	44(2)	42(2)	35(2)	-9(1)	6(1)	8(1)
F(20)	38(2)	27(2)	33(2)	-7(1)	-1(1)	-3(1)
F(22)	48(2)	37(2)	32(2)	2(1)	-3(1)	11(1)
F(23)	65(2)	40(2)	56(2)	-2(2)	-12(2)	24(2)
F(24)	40(2)	59(2)	68(2)	-25(2)	2(2)	16(2)
F(25)	42(2)	77(2)	47(2)	-10(2)	14(2)	-1(2)
F(26)	39(2)	44(2)	37(2)	5(1)	4(1)	0(1)
F(28)	39(2)	33(2)	43(2)	-7(1)	-9(1)	4(1)
F(29)	39(2)	46(2)	63(2)	6(2)	-3(2)	16(1)
F(30)	36(2)	79(2)	62(2)	6(2)	-22(2)	11(2)
F(31)	45(2)	81(3)	44(2)	-15(2)	-20(2)	-1(2)
F(32)	38(2)	42(2)	37(2)	-11(1)	-8(1)	3(1)
F(34)	34(2)	36(2)	37(2)	10(1)	-10(1)	-2(1)
F(35)	31(2)	54(2)	50(2)	3(2)	-12(1)	-6(1)

F(36)	36(2)	39(2)	59(2)	-3(2)	1(1)	-15(1)
F(37)	47(2)	35(2)	53(2)	14(2)	-3(1)	-9(1)
F(38)	39(2)	40(2)	37(2)	14(1)	-13(1)	-6(1)
C(15)	22(2)	20(3)	30(3)	5(2)	-4(2)	1(2)
C(16)	30(3)	28(3)	23(2)	-3(2)	-6(2)	5(2)
C(17)	29(3)	24(3)	36(3)	10(2)	-6(2)	-5(2)
C(18)	26(2)	34(3)	26(3)	8(2)	2(2)	5(2)
C(19)	27(2)	27(3)	30(3)	-5(2)	-4(2)	8(2)
C(20)	26(2)	16(3)	30(3)	-2(2)	-2(2)	1(2)
C(21)	23(2)	30(3)	24(2)	-8(2)	-5(2)	-5(2)
C(22)	34(3)	29(3)	30(3)	-6(2)	-7(2)	2(2)
C(23)	37(3)	29(3)	38(3)	-7(2)	-8(2)	5(2)
C(24)	26(3)	44(3)	49(3)	-21(3)	-2(2)	4(2)
C(25)	24(3)	46(3)	34(3)	-12(3)	4(2)	-1(2)
C(26)	28(3)	31(3)	36(3)	-3(2)	-1(2)	-7(2)
C(27)	30(3)	26(3)	20(2)	3(2)	4(2)	0(2)
C(28)	30(3)	31(3)	28(3)	-1(2)	-3(2)	-4(2)
C(29)	29(3)	34(3)	39(3)	7(3)	1(2)	4(2)
C(30)	25(3)	51(4)	41(3)	13(3)	-10(2)	5(2)
C(31)	33(3)	49(3)	28(3)	0(3)	-11(2)	-9(3)
C(32)	30(3)	33(3)	31(3)	2(2)	6(2)	1(2)
C(33)	23(2)	25(3)	24(2)	-3(2)	-1(2)	2(2)
C(34)	24(2)	23(3)	29(3)	2(2)	2(2)	-1(2)
C(35)	22(2)	36(3)	27(3)	-3(2)	-3(2)	4(2)
C(36)	27(3)	35(3)	38(3)	-11(2)	2(2)	-12(2)
C(37)	33(3)	31(3)	30(3)	-1(2)	-1(2)	-2(2)
C(38)	24(2)	32(3)	28(3)	0(2)	-4(2)	4(2)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **6.C₆H₅Cl**.

	x	y	z	U(eq)
H(1A)	2924	8384	1863	94
H(1B)	2131	7763	1790	94
H(1C)	2895	7028	1742	94
H(2)	4395	7051	2787	51
H(3A)	4383	4871	2765	74
H(3B)	5089	5409	2598	74
H(3C)	4367	4939	2421	74
H(4A)	4182	6977	2172	109
H(4B)	4929	7461	2330	109
H(4C)	4154	8188	2360	109
H(6)	3968	6090	3116	57
H(7)	3681	5477	3548	76
H(8)	2557	5084	3743	78
H(9)	1444	5271	3518	64
H(10)	1177	5813	3075	56
H(12)	765	6902	2757	54
H(13A)	793	4920	2355	92
H(13B)	67	5357	2527	92
H(13C)	760	4749	2697	92
H(14A)	1064	8141	2356	126
H(14B)	245	7545	2330	126
H(14C)	927	6997	2150	126
H(1A1)	4942	-3844	5386	73
H(1A2)	4745	-2951	5646	73
H(1A3)	5040	-2413	5348	73
H(2A)	1848	-4077	5708	40
H(3A1)	2316	-1704	5896	68
H(3A2)	1762	-2576	6069	68
H(3A3)	1494	-1993	5769	68
H(4A1)	3151	-4613	5776	57

H(4A2)	2780	-4205	6073	57
H(4A3)	3315	-3291	5903	57
H(6A)	1030	-3192	5453	58
H(7A)	23	-2942	5189	39
H(8A)	-118	-2444	4723	56
H(9A)	837	-2090	4424	66
H(10A)	2046	-2123	4493	49
H(12A)	3168	-1445	4524	43
H(13D)	4297	-1307	4804	70
H(13E)	4506	-1866	4497	70
H(13F)	4439	-2731	4772	70
H(14D)	3530	-3991	4471	141
H(14E)	3539	-3048	4210	141
H(14F)	2759	-3411	4355	141
H(1B1)	2980	-6958	5162	79
H(1B2)	3309	-6535	5468	79
H(1B3)	3830	-6491	5190	79
H(2B)	2932	-1966	5761	45
H(3B1)	1592	-2230	5764	80
H(3B2)	1963	-2713	6058	80
H(3B3)	1703	-3652	5814	80
H(4B1)	3015	-4566	5804	57
H(4B2)	3325	-3636	6042	57
H(4B3)	3726	-3728	5736	57
H(6B)	2290	-797	5539	53
H(7B)	1922	884	5336	49
H(8B)	1730	1385	4876	83
H(9B)	1891	157	4501	75
H(10B)	2251	-1723	4475	60
H(12B)	2212	-3588	4402	47
H(13G)	3419	-2503	4384	53
H(13H)	3344	-3556	4148	53
H(13I)	3832	-3774	4436	53
H(14G)	3199	-5537	4578	84
H(14H)	2662	-5545	4299	84
H(14I)	2305	-5608	4614	84

H(101)	3436	774	4806	76
H(102)	2355	1423	4541	83
H(103)	1178	1189	4733	98
H(104)	1107	437	5232	100
H(105)	1974	-87	5445	99
H(201)	833	-4552	4576	73
H(202)	359	-2704	4410	92
H(203)	10	-1157	4717	81
H(204)	248	-1325	5221	94
H(205)	707	-3430	5419	68
H(301)	4570	-1898	4709	84
H(302)	4229	185	4682	87
H(303)	3925	1280	5111	79
H(304)	3963	273	5547	66
H(305)	4423	-1752	5594	49
H(401)	2152	-6020	5335	61
H(402)	975	-5921	5091	66
H(403)	914	-6050	4580	86
H(404)	2046	-6193	4336	88
H(405)	3183	-6310	4570	70

VI. X-ray Crystallographic Analysis of $(i\text{Pr}_2\text{-ATT})\text{In}(\text{C}_6\text{F}_5)_2$ (9).

Crystallographic Experimental Section

Data Collection

A yellow crystal with approximate dimensions $0.45 \times 0.43 \times 0.27 \text{ mm}^3$ 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 173(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 ($\lambda = 0.71073 \text{ \AA}$) 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 8166 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 1.8 hemisphere to a resolution of $0.80 \text{ \AA}$. A total of 11469 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 consistent for space groups $Pnma$ and $Pna2_1$ but only the latter, non-centrosymmetric space group $Pna2_1$ 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. The final least-squares refinement of 347 parameters against 4577 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0169 and 0.0376, respectively. The final difference Fourier map was featureless.

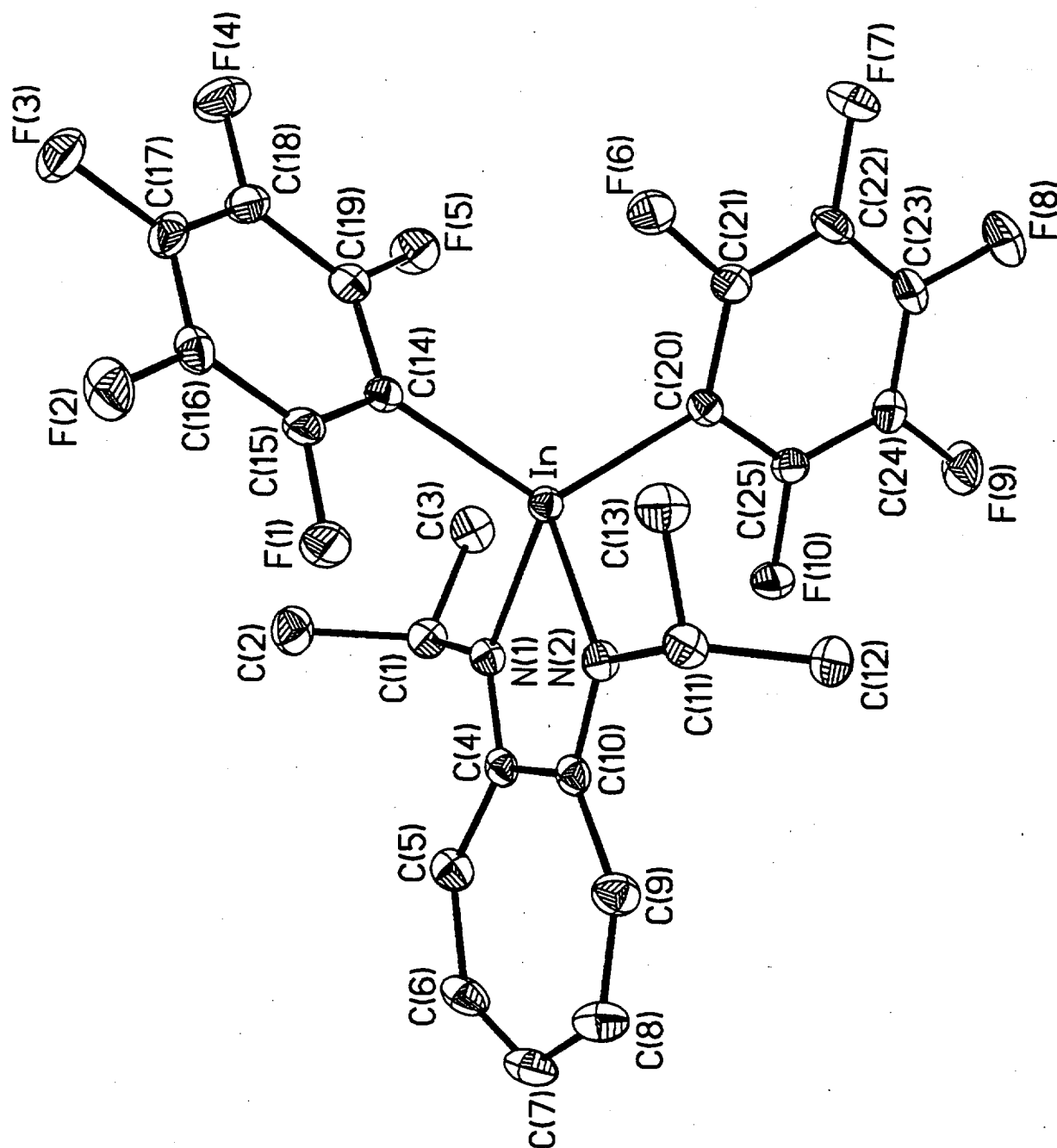
The ORTEP diagrams were drawn with 30% probability ellipsoids.

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 **9**

Identification code	jor26	
Empirical formula	C ₂₅ H ₁₉ F ₁₀ In N ₂	
Formula weight	652.24	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2 ₁	
Unit cell dimensions	a = 16.3299(10) Å	α = 90°
	b = 17.6995(11) Å	β = 90°
	c = 8.5897(5) Å	γ = 90°
Volume	2482.7(3) Å ³	
Z	4	
Density (calculated)	1.745 Mg/m ³	
Absorption coefficient	1.045 mm ⁻¹	
F(000)	1288	
Crystal size	0.45 x 0.43 x 0.27 mm ³	
Theta range for data collection	1.70 to 26.37°	
Index ranges	-19 ≤ h ≤ 20, -13 ≤ k ≤ 22, -10 ≤ l ≤ 10	
Reflections collected	11469	
Independent reflections	4577 [R(int) = 0.0176]	
Completeness to theta = 26.37°	99.8 %	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.7657 and 0.6507	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4577 / 1 / 347	
Goodness-of-fit on F ²	0.988	
Final R indices [I > 2σ(I)]	R1 = 0.0169, wR2 = 0.0376	
R indices (all data)	R1 = 0.0199, wR2 = 0.0384	
Absolute structure parameter	0.005(12)	
Largest diff. peak and hole	0.242 and -0.357 e.Å ⁻³	



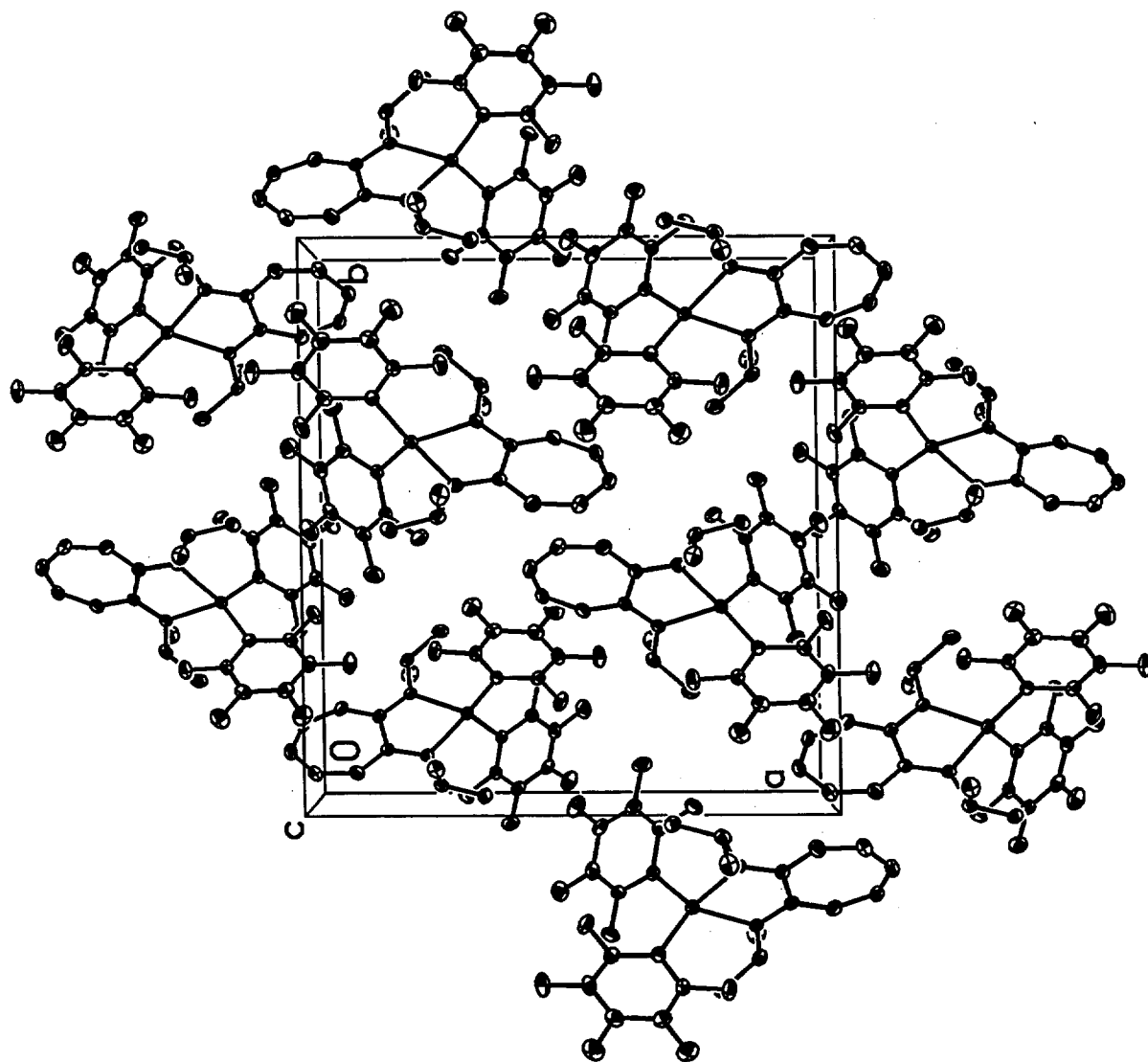


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9**.U(eq) is defined as one third of the trace of the orthogonalized $U^{\dagger}$ tensor.

	x	y	z	U(eq)
In	2147(1)	6438(1)	3115(1)	25(1)
F(1)	2229(1)	4810(1)	1265(2)	42(1)
F(2)	1319(1)	4171(1)	-966(2)	50(1)
F(3)	65(1)	4949(1)	-2286(2)	55(1)
F(4)	-258(1)	6387(1)	-1366(2)	54(1)
F(5)	665(1)	7040(1)	853(2)	44(1)
F(6)	208(1)	6673(1)	4036(2)	48(1)
F(7)	-572(1)	7549(1)	6130(2)	55(1)
F(8)	306(1)	8456(1)	8075(3)	58(1)
F(9)	1949(1)	8508(1)	7857(2)	54(1)
F(10)	2740(1)	7667(1)	5703(2)	45(1)
N(1)	3325(1)	6796(1)	2357(2)	26(1)
N(2)	2958(1)	5687(1)	4283(2)	27(1)
C(1)	3412(1)	7415(1)	1217(3)	33(1)
C(2)	3401(2)	7103(2)	-441(3)	47(1)
C(3)	2712(2)	7969(1)	1450(3)	41(1)
C(4)	3955(1)	6385(1)	2847(3)	26(1)
C(5)	4755(1)	6512(1)	2244(3)	36(1)
C(6)	5519(1)	6238(1)	2676(3)	41(1)
C(7)	5742(1)	5745(1)	3824(3)	45(1)
C(8)	5204(1)	5364(1)	4798(3)	46(1)
C(9)	4358(1)	5378(1)	4843(3)	38(1)
C(10)	3758(1)	5792(1)	4026(2)	26(1)
C(11)	2656(1)	5162(1)	5469(3)	33(1)
C(12)	2726(2)	5520(2)	7073(3)	44(1)
C(13)	1779(2)	4950(2)	5122(3)	39(1)
C(14)	1466(1)	5943(1)	1188(2)	27(1)
C(15)	1601(1)	5217(1)	668(3)	30(1)
C(16)	1144(1)	4874(1)	-479(3)	34(1)
C(17)	514(1)	5269(1)	-1157(3)	36(1)
C(18)	357(1)	5998(1)	-694(3)	35(1)

C(19)	831(1)	6318(1)	448(3)	30(1)
C(20)	1504(1)	7139(1)	4777(2)	27(1)
C(21)	661(2)	7135(1)	4959(3)	32(1)
C(22)	249(1)	7565(1)	6036(3)	37(1)
C(23)	686(1)	8023(1)	7007(3)	38(1)
C(24)	1531(1)	8052(1)	6895(3)	35(1)
C(25)	1915(1)	7618(1)	5794(3)	30(1)

Table 2. Bond lengths [Å] and angles [°] for 9.

In-N(1)	2.1260(17)
In-N(2)	2.1286(17)
In-C(20)	2.164(2)
In-C(14)	2.178(2)
F(1)-C(15)	1.354(3)
F(2)-C(16)	1.343(2)
F(3)-C(17)	1.341(2)
F(4)-C(18)	1.349(3)
F(5)-C(19)	1.351(2)
F(6)-C(21)	1.358(3)
F(7)-C(22)	1.344(2)
F(8)-C(23)	1.347(3)
F(9)-C(24)	1.342(3)
F(10)-C(25)	1.352(2)
N(1)-C(4)	1.330(3)
N(1)-C(1)	1.475(3)
N(2)-C(10)	1.337(2)
N(2)-C(11)	1.465(3)
C(1)-C(3)	1.520(3)
C(1)-C(2)	1.527(3)
C(4)-C(5)	1.423(3)
C(4)-C(10)	1.493(3)
C(5)-C(6)	1.390(3)
C(6)-C(7)	1.365(4)
C(7)-C(8)	1.389(4)
C(8)-C(9)	1.381(3)
C(9)-C(10)	1.411(3)
C(11)-C(13)	1.510(3)
C(11)-C(12)	1.521(4)
C(14)-C(15)	1.378(3)
C(14)-C(19)	1.386(3)
C(15)-C(16)	1.377(3)
C(16)-C(17)	1.373(3)
C(17)-C(18)	1.375(3)

C(18)-C(19)	1.372(3)
C(20)-C(21)	1.384(3)
C(20)-C(25)	1.390(3)
C(21)-C(22)	1.374(3)
C(22)-C(23)	1.365(3)
C(23)-C(24)	1.384(3)
C(24)-C(25)	1.370(3)
N(1)-In-N(2)	76.59(6)
N(1)-In-C(20)	118.09(7)
N(2)-In-C(20)	110.45(7)
N(1)-In-C(14)	110.43(7)
N(2)-In-C(14)	115.10(7)
C(20)-In-C(14)	118.94(8)
C(4)-N(1)-C(1)	122.82(17)
C(4)-N(1)-In	116.11(14)
C(1)-N(1)-In	120.75(14)
C(10)-N(2)-C(11)	122.18(17)
C(10)-N(2)-In	116.28(14)
C(11)-N(2)-In	120.95(13)
N(1)-C(1)-C(3)	108.61(18)
N(1)-C(1)-C(2)	110.49(19)
C(3)-C(1)-C(2)	110.3(2)
N(1)-C(4)-C(5)	120.6(2)
N(1)-C(4)-C(10)	115.63(17)
C(5)-C(4)-C(10)	123.82(19)
C(6)-C(5)-C(4)	132.2(2)
C(7)-C(6)-C(5)	130.9(2)
C(6)-C(7)-C(8)	125.3(2)
C(9)-C(8)-C(7)	129.8(3)
C(8)-C(9)-C(10)	133.6(2)
N(2)-C(10)-C(9)	121.6(2)
N(2)-C(10)-C(4)	114.86(18)
C(9)-C(10)-C(4)	123.50(19)
N(2)-C(11)-C(13)	109.89(18)
N(2)-C(11)-C(12)	109.9(2)

C(13)-C(11)-C(12)	110.7(2)
C(15)-C(14)-C(19)	114.68(19)
C(15)-C(14)-In	122.68(16)
C(19)-C(14)-In	122.54(16)
F(1)-C(15)-C(16)	116.5(2)
F(1)-C(15)-C(14)	119.6(2)
C(16)-C(15)-C(14)	123.8(2)
F(2)-C(16)-C(17)	119.9(2)
F(2)-C(16)-C(15)	121.1(2)
C(17)-C(16)-C(15)	119.0(2)
F(3)-C(17)-C(16)	120.1(2)
F(3)-C(17)-C(18)	120.3(2)
C(16)-C(17)-C(18)	119.6(2)
F(4)-C(18)-C(19)	121.0(2)
F(4)-C(18)-C(17)	119.7(2)
C(19)-C(18)-C(17)	119.3(2)
F(5)-C(19)-C(18)	117.5(2)
F(5)-C(19)-C(14)	119.03(19)
C(18)-C(19)-C(14)	123.5(2)
C(21)-C(20)-C(25)	114.3(2)
C(21)-C(20)-In	123.68(17)
C(25)-C(20)-In	121.95(14)
F(6)-C(21)-C(22)	117.3(2)
F(6)-C(21)-C(20)	118.6(2)
C(22)-C(21)-C(20)	124.1(2)
F(7)-C(22)-C(23)	119.9(2)
F(7)-C(22)-C(21)	121.2(2)
C(23)-C(22)-C(21)	118.9(2)
F(8)-C(23)-C(22)	120.8(2)
F(8)-C(23)-C(24)	119.1(2)
C(22)-C(23)-C(24)	120.1(2)
F(9)-C(24)-C(25)	122.0(2)
F(9)-C(24)-C(23)	119.1(2)
C(25)-C(24)-C(23)	118.9(2)
F(10)-C(25)-C(24)	117.4(2)
F(10)-C(25)-C(20)	118.98(19)

C(24)-C(25)-C(20)

123.7(2)

Table 3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 9. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ln	24(1)	25(1)	25(1)	0(1)	1(1)	-2(1)
F(1)	42(1)	37(1)	47(1)	-5(1)	-5(1)	12(1)
F(2)	59(1)	37(1)	55(1)	-19(1)	6(1)	-8(1)
F(3)	51(1)	73(1)	40(1)	-11(1)	-11(1)	-20(1)
F(4)	42(1)	67(1)	53(1)	10(1)	-18(1)	5(1)
F(5)	46(1)	31(1)	54(1)	-4(1)	-6(1)	10(1)
F(6)	34(1)	61(1)	49(1)	-12(1)	1(1)	-17(1)
F(7)	28(1)	81(1)	56(1)	1(1)	12(1)	3(1)
F(8)	62(1)	65(1)	46(1)	-15(1)	20(1)	10(1)
F(9)	62(1)	59(1)	42(2)	-22(1)	2(1)	-11(1)
F(10)	27(1)	64(1)	45(1)	-12(1)	-2(1)	-5(1)
N(1)	26(1)	24(1)	27(1)	0(1)	3(1)	-4(1)
N(2)	30(1)	25(1)	25(1)	2(1)	2(1)	-1(1)
C(1)	31(1)	33(1)	35(1)	6(1)	3(1)	-9(1)
C(2)	50(2)	62(2)	31(1)	6(1)	7(1)	-7(1)
C(3)	49(1)	29(1)	44(2)	6(1)	4(1)	-2(1)
C(4)	26(1)	25(1)	27(2)	-8(1)	3(1)	-4(1)
C(5)	32(1)	33(1)	42(1)	-3(1)	5(1)	-7(1)
C(6)	25(1)	40(1)	57(2)	-12(1)	10(1)	-5(1)
C(7)	26(1)	43(1)	67(2)	-14(1)	1(1)	5(1)
C(8)	34(1)	41(2)	61(2)	2(1)	-5(1)	8(1)
C(9)	37(1)	36(1)	43(1)	6(1)	2(1)	4(1)
C(10)	28(1)	25(1)	26(1)	-6(1)	2(1)	-1(1)
C(11)	35(1)	30(1)	33(1)	10(1)	5(1)	4(1)
C(12)	47(1)	57(2)	29(1)	7(1)	1(1)	4(1)
C(13)	36(1)	37(2)	45(2)	17(1)	4(1)	-4(1)
C(14)	23(1)	30(1)	28(1)	-1(1)	3(1)	-2(1)
C(15)	24(1)	35(1)	30(1)	2(1)	4(1)	0(1)
C(16)	37(1)	32(1)	33(1)	-8(1)	9(1)	-8(1)
C(17)	33(1)	46(1)	29(1)	-4(1)	0(1)	-15(1)
C(18)	27(1)	45(1)	32(1)	6(1)	-2(1)	-2(1)

C(19)	31(1)	28(1)	32(1)	2(1)	3(1)	-1(1)
C(20)	27(1)	27(1)	27(1)	1(1)	3(1)	0(1)
C(21)	32(1)	32(1)	32(1)	3(1)	0(1)	-5(1)
C(22)	27(1)	48(2)	36(1)	8(1)	11(1)	4(1)
C(23)	44(1)	40(1)	30(1)	-4(1)	12(1)	5(1)
C(24)	43(1)	35(1)	26(1)	-3(1)	0(1)	-5(1)
C(25)	26(1)	35(1)	29(1)	3(1)	-1(1)	0(1)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **9**.

	x	y	z	U(eq)
H(1)	3943	7681	1402	39
H(2A)	3828	6719	-552	71
H(2B)	3502	7515	-1179	71
H(2C)	2865	6877	-655	71
H(3A)	2190	7716	1230	61
H(3B)	2780	8398	742	61
H(3C)	2713	8149	2529	61
H(5)	4769	6849	1383	43
H(6)	5962	6426	2071	49
H(7)	6311	5656	3967	54
H(8)	5456	5045	5548	55
H(9)	4134	5035	5580	46
H(11)	2999	4694	5444	39
H(12A)	3289	5695	7237	66
H(12B)	2586	5145	7870	66
H(12C)	2350	5949	7146	66
H(13A)	1433	5401	5188	59
H(13B)	1591	4575	5882	59
H(13C)	1743	4737	4072	59

VII. X-ray Crystallographic Analysis of $[(^i\text{Pr}_2\text{-ATI})\text{In}(\text{Me})(\text{NMe}_2\text{Ph})][\text{B}(\text{C}_6\text{F}_5)_4]$ (**10**).

Crystallographic Experimental Section

Data Collection

A yellow crystal with approximate dimensions $0.41 \times 0.39 \times 0.39 \text{ mm}^3$ 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 ($\lambda = 0.71073 \text{ \AA}$) 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 77 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 7424 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 $0.80 \text{ \AA}$. A total of 33129 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. The isopropyl group on atom N(2) is equally disordered over two positions and was refined with an idealized geometry. The final least-squares refinement of 670 parameters against 9111 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0253 and 0.0622, respectively. The final difference Fourier map was featureless.

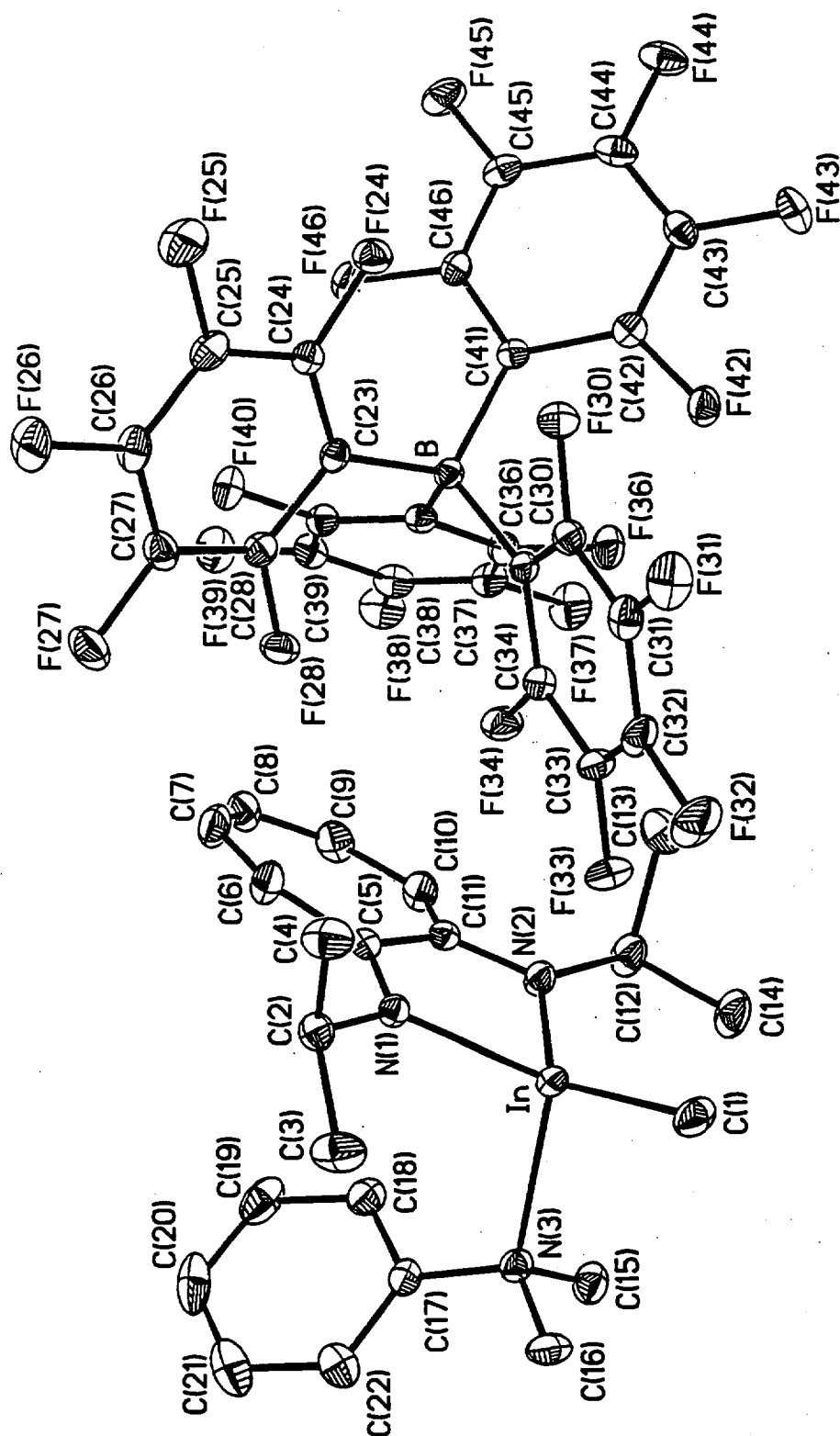
The ORTEP diagrams were drawn with 30% probability ellipsoids.

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 **10**

Identification code	jor24	
Empirical formula	C ₄₆ H ₃₃ B F ₂₀ In N ₃	
Formula weight	1133.38	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /c	
Unit cell dimensions	a = 12.1883(9) Å	α = 90°
	b = 20.9248(16) Å	β = 93.187(1)°
	c = 17.5691(13) Å	γ = 90°
Volume	4473.9(6) Å ³	
Z	4	
Density (calculated)	1.683 Mg/m ³	
Absorption coefficient	0.650 mm ⁻¹	
F(000)	2256	
Crystal size	0.41 x 0.39 x 0.39 mm ³	
Theta range for data collection	1.95 to 26.37°	
Index ranges	-15 ≤ h ≤ 15, 0 ≤ k ≤ 26, 0 ≤ l ≤ 21	
Reflections collected	33129	
Independent reflections	9111 [R(int) = 0.0162]	
Completeness to theta = 26.37°	99.7 %	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.7855 and 0.7763	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9111 / 24 / 670	
Goodness-of-fit on F ²	1.024	
Final R indices [I > 2σ(I)]	R1 = 0.0253, wR2 = 0.0622	
R indices (all data)	R1 = 0.0341, wR2 = 0.0665	
Largest diff. peak and hole	0.739 and -0.762 e.Å ⁻³	



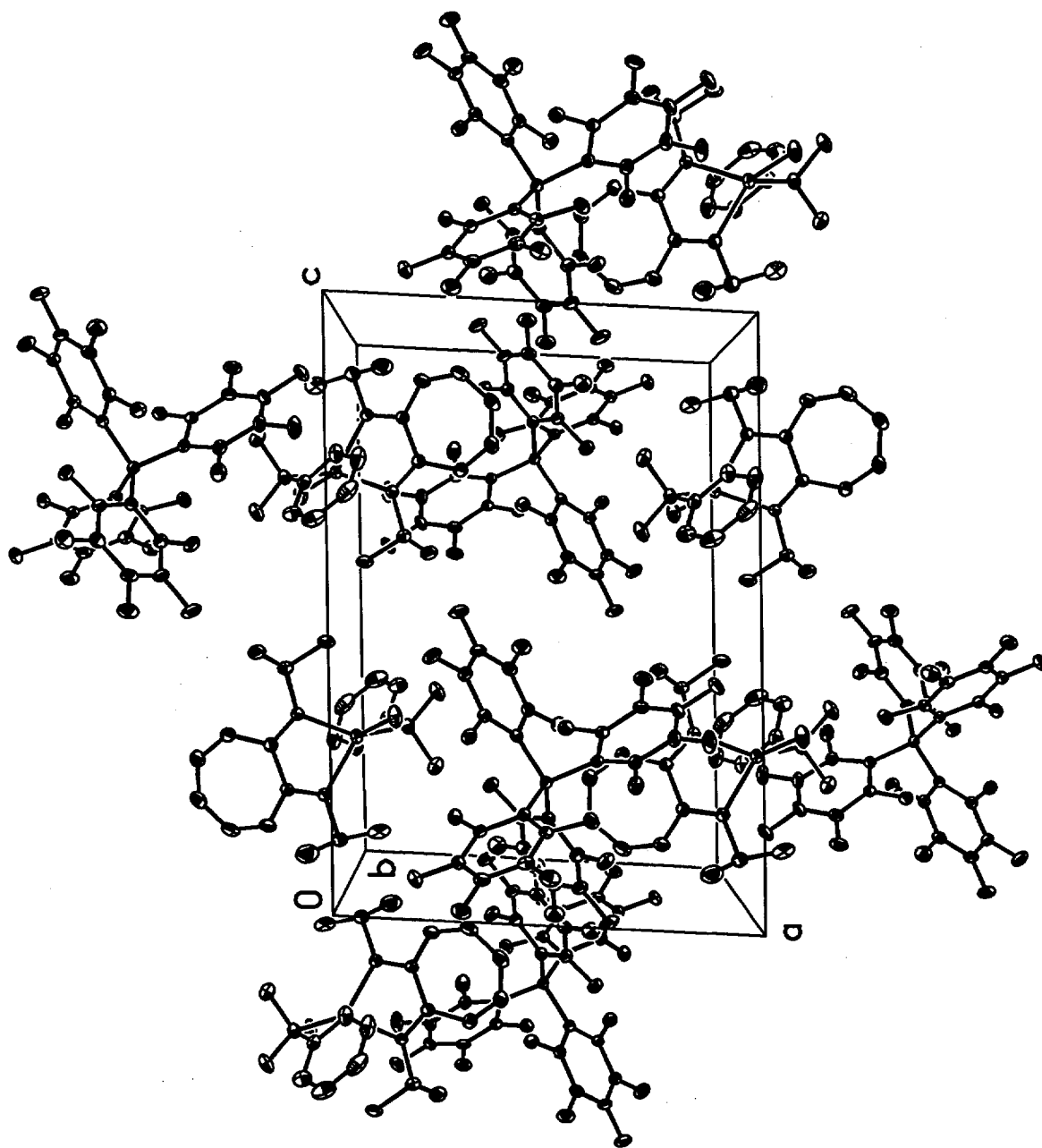


Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **10**.U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ln	10324(1)	1321(1)	7649(1)	26(1)
F(24)	3184(1)	3769(1)	7889(1)	31(1)
F(25)	2340(1)	3465(1)	9192(1)	44(1)
F(26)	2956(1)	2381(1)	9951(1)	46(1)
F(27)	4498(1)	1602(1)	9370(1)	44(1)
F(28)	5389(1)	1901(1)	8062(1)	34(1)
F(30)	5492(1)	4103(1)	8134(1)	30(1)
F(31)	7305(1)	4325(1)	9016(1)	43(1)
F(32)	9102(1)	3559(1)	8927(1)	54(1)
F(33)	9022(1)	2561(1)	7930(1)	52(1)
F(34)	7226(1)	2292(1)	7104(1)	39(1)
F(36)	6419(1)	3048(1)	5869(1)	37(1)
F(37)	6528(1)	2198(1)	4745(1)	48(1)
F(38)	5221(1)	1139(1)	4712(1)	47(1)
F(39)	3790(1)	961(1)	5827(1)	44(1)
F(40)	3665(1)	1792(1)	6951(1)	34(1)
F(42)	6034(1)	4310(1)	6651(1)	33(1)
F(43)	5033(1)	5183(1)	5783(1)	41(1)
F(44)	2961(1)	4980(1)	5159(1)	42(1)
F(45)	1862(1)	3899(1)	5520(1)	43(1)
F(46)	2803(1)	3043(1)	6487(1)	31(1)
N(1)	8811(1)	945(1)	7970(1)	26(1)
N(2)	9470(1)	1197(1)	6585(1)	31(1)
N(3)	11577(1)	439(1)	7818(1)	30(1)
B	5025(2)	3032(1)	7137(1)	21(1)
C(1)	11349(2)	2075(1)	8072(2)	44(1)
C(2)	8522(2)	869(1)	8772(1)	32(1)
C(3)	9552(2)	754(2)	9273(1)	49(1)
C(4)	7901(2)	1448(1)	9050(1)	47(1)
C(5)	8104(2)	792(1)	7392(1)	26(1)
C(6)	7014(2)	597(1)	7520(1)	38(1)

C(7)	6190(2)	328(1)	7054(2)	44(1)
C(8)	6171(2)	170(1)	6295(2)	43(1)
C(9)	6986(2)	306(1)	5815(1)	43(1)
C(10)	7972(2)	632(1)	5954(1)	39(1)
C(11)	8508(2)	880(1)	6616(1)	28(1)
C(12)	9853(2)	1428(1)	5839(1)	50(1)
C(13)	9099(4)	1996(2)	5631(3)	67(2)
C(14)	10881(2)	1818(2)	6058(4)	63(3)
C(13A)	10439(2)	876(2)	5445(3)	58(2)
C(14A)	10647(8)	1983(4)	5898(5)	86(3)
C(15)	12249(2)	413(1)	7138(2)	41(1)
C(16)	12329(2)	609(1)	8483(2)	41(1)
C(17)	11010(2)	-172(1)	7911(1)	30(1)
C(18)	10165(2)	-326(1)	7380(2)	39(1)
C(19)	9557(2)	-880(1)	7466(2)	53(1)
C(20)	9810(3)	-1284(1)	8070(2)	60(1)
C(21)	10677(3)	-1145(1)	8576(2)	58(1)
C(22)	11275(2)	-588(1)	8503(1)	42(1)
C(23)	4327(2)	2843(1)	7888(1)	22(1)
C(24)	3552(2)	3222(1)	8223(1)	24(1)
C(25)	3101(2)	3079(1)	8909(1)	29(1)
C(26)	3416(2)	2535(1)	9296(1)	31(1)
C(27)	4183(2)	2138(1)	8996(1)	30(1)
C(28)	4619(2)	2303(1)	8313(1)	26(1)
C(29)	6246(2)	3195(1)	7555(1)	23(1)
C(30)	6355(2)	3702(1)	8063(1)	25(1)
C(31)	7281(2)	3831(1)	8522(1)	30(1)
C(32)	8188(2)	3445(1)	8477(1)	36(1)
C(33)	8137(2)	2944(1)	7981(1)	34(1)
C(34)	7186(2)	2819(1)	7544(1)	29(1)
C(35)	5070(2)	2460(1)	6492(1)	24(1)
C(36)	5759(2)	2530(1)	5892(1)	28(1)
C(37)	5831(2)	2097(1)	5304(1)	33(1)
C(38)	5178(2)	1562(1)	5283(1)	33(1)
C(39)	4461(2)	1476(1)	5848(1)	31(1)
C(40)	4419(2)	1919(1)	6429(1)	27(1)

C(41)	4467(2)	3627(1)	6633(1)	22(1)
C(42)	4980(2)	4184(1)	6411(1)	25(1)
C(43)	4489(2)	4643(1)	5941(1)	28(1)
C(44)	3444(2)	4546(1)	5636(1)	31(1)
C(45)	2888(2)	4000(1)	5825(1)	29(1)
C(46)	3400(2)	3565(1)	6314(1)	25(1)

Table 2. Bond lengths [Å] and angles [°] for 10.

In-N(2)	2.1042(18)
In-N(1)	2.1115(16)
In-C(1)	2.121(2)
In-N(3)	2.4048(17)
F(24)-C(24)	1.351(2)
F(25)-C(25)	1.346(2)
F(26)-C(26)	1.346(2)
F(27)-C(27)	1.347(2)
F(28)-C(28)	1.353(2)
F(30)-C(30)	1.356(2)
F(31)-C(31)	1.348(2)
F(32)-C(32)	1.351(2)
F(33)-C(33)	1.351(2)
F(34)-C(34)	1.350(2)
F(36)-C(36)	1.352(2)
F(37)-C(37)	1.351(2)
F(38)-C(38)	1.342(2)
F(39)-C(39)	1.352(2)
F(40)-C(40)	1.359(2)
F(42)-C(42)	1.356(2)
F(43)-C(43)	1.348(2)
F(44)-C(44)	1.349(2)
F(45)-C(45)	1.349(2)
F(46)-C(46)	1.356(2)
N(1)-C(5)	1.333(3)
N(1)-C(2)	1.479(3)
N(2)-C(11)	1.351(3)
N(2)-C(12)	1.495(3)
N(3)-C(17)	1.467(3)
N(3)-C(15)	1.486(3)
N(3)-C(16)	1.487(3)
B-C(35)	1.651(3)
B-C(41)	1.653(3)
B-C(23)	1.656(3)

B-C(29)	1.657(3)
C(2)-C(3)	1.513(3)
C(2)-C(4)	1.523(3)
C(5)-C(6)	1.419(3)
C(5)-C(11)	1.487(3)
C(6)-C(7)	1.380(3)
C(7)-C(8)	1.374(4)
C(8)-C(9)	1.368(4)
C(9)-C(10)	1.391(3)
C(10)-C(11)	1.402(3)
C(12)-C(14A)	1.511(2)
C(12)-C(14)	1.526(2)
C(12)-C(13)	1.534(2)
C(12)-C(13A)	1.542(2)
C(17)-C(22)	1.379(3)
C(17)-C(18)	1.389(3)
C(18)-C(19)	1.389(3)
C(19)-C(20)	1.377(4)
C(20)-C(21)	1.374(5)
C(21)-C(22)	1.384(4)
C(23)-C(24)	1.390(3)
C(23)-C(28)	1.391(3)
C(24)-C(25)	1.386(3)
C(25)-C(26)	1.370(3)
C(26)-C(27)	1.377(3)
C(27)-C(28)	1.381(3)
C(29)-C(34)	1.390(3)
C(29)-C(30)	1.390(3)
C(30)-C(31)	1.377(3)
C(31)-C(32)	1.376(3)
C(32)-C(33)	1.361(3)
C(33)-C(34)	1.379(3)
C(35)-C(40)	1.384(3)
C(35)-C(36)	1.392(3)
C(36)-C(37)	1.379(3)
C(37)-C(38)	1.372(3)

C(38)-C(39)	1.371(3)
C(39)-C(40)	1.382(3)
C(41)-C(42)	1.389(3)
C(41)-C(46)	1.393(3)
C(42)-C(43)	1.381(3)
C(43)-C(44)	1.369(3)
C(44)-C(45)	1.379(3)
C(45)-C(46)	1.377(3)
N(2)-In-N(1)	78.18(6)
N(2)-In-C(1)	131.03(9)
N(1)-In-C(1)	133.62(9)
N(2)-In-N(3)	107.10(7)
N(1)-In-N(3)	103.79(6)
C(1)-In-N(3)	99.79(8)
C(5)-N(1)-C(2)	121.45(17)
C(5)-N(1)-In	114.99(13)
C(2)-N(1)-In	123.54(13)
C(11)-N(2)-C(12)	120.54(18)
C(11)-N(2)-In	114.36(13)
C(12)-N(2)-In	125.10(13)
C(17)-N(3)-C(15)	110.02(16)
C(17)-N(3)-C(16)	113.26(18)
C(15)-N(3)-C(16)	107.25(18)
C(17)-N(3)-In	112.55(12)
C(15)-N(3)-In	107.62(13)
C(16)-N(3)-In	105.82(12)
C(35)-B-C(41)	101.90(15)
C(35)-B-C(23)	114.33(15)
C(41)-B-C(23)	113.05(15)
C(35)-B-C(29)	112.94(15)
C(41)-B-C(29)	114.52(16)
C(23)-B-C(29)	100.68(15)
N(1)-C(2)-C(3)	109.73(17)
N(1)-C(2)-C(4)	111.68(18)
C(3)-C(2)-C(4)	110.5(2)

N(1)-C(5)-C(6)	121.24(19)
N(1)-C(5)-C(11)	115.86(17)
C(6)-C(5)-C(11)	122.78(19)
C(7)-C(6)-C(5)	132.8(2)
C(8)-C(7)-C(6)	130.3(2)
C(9)-C(8)-C(7)	125.1(2)
C(8)-C(9)-C(10)	130.0(2)
C(9)-C(10)-C(11)	133.3(2)
N(2)-C(11)-C(10)	120.91(19)
N(2)-C(11)-C(5)	115.49(18)
C(10)-C(11)-C(5)	123.53(19)
N(2)-C(12)-C(14A)	114.7(4)
N(2)-C(12)-C(14)	104.1(3)
C(14A)-C(12)-C(14)	19.7(4)
N(2)-C(12)-C(13)	104.3(3)
C(14A)-C(12)-C(13)	78.1(5)
C(14)-C(12)-C(13)	96.7(3)
N(2)-C(12)-C(13A)	109.1(2)
C(14A)-C(12)-C(13A)	107.1(5)
C(14)-C(12)-C(13A)	96.80(12)
C(13)-C(12)-C(13A)	139.4(3)
C(22)-C(17)-C(18)	119.6(2)
C(22)-C(17)-N(3)	122.8(2)
C(18)-C(17)-N(3)	117.6(2)
C(17)-C(18)-C(19)	120.0(3)
C(20)-C(19)-C(18)	119.9(3)
C(21)-C(20)-C(19)	119.9(2)
C(20)-C(21)-C(22)	120.6(3)
C(17)-C(22)-C(21)	119.9(3)
C(24)-C(23)-C(28)	113.29(17)
C(24)-C(23)-B	126.36(17)
C(28)-C(23)-B	119.65(16)
F(24)-C(24)-C(25)	114.98(17)
F(24)-C(24)-C(23)	121.14(17)
C(25)-C(24)-C(23)	123.88(19)
F(25)-C(25)-C(26)	119.74(18)

F(25)-C(25)-C(24)	120.41(19)
C(26)-C(25)-C(24)	119.84(19)
F(26)-C(26)-C(25)	120.26(19)
F(26)-C(26)-C(27)	120.5(2)
C(25)-C(26)-C(27)	119.22(18)
F(27)-C(27)-C(26)	119.81(18)
F(27)-C(27)-C(28)	121.18(19)
C(26)-C(27)-C(28)	119.01(19)
F(28)-C(28)-C(27)	115.87(18)
F(28)-C(28)-C(23)	119.38(17)
C(27)-C(28)-C(23)	124.75(18)
C(34)-C(29)-C(30)	113.00(18)
C(34)-C(29)-B	126.77(18)
C(30)-C(29)-B	119.55(16)
F(30)-C(30)-C(31)	116.07(18)
F(30)-C(30)-C(29)	119.01(17)
C(31)-C(30)-C(29)	124.92(19)
F(31)-C(31)-C(32)	119.9(2)
F(31)-C(31)-C(30)	121.0(2)
C(32)-C(31)-C(30)	119.1(2)
F(32)-C(32)-C(33)	121.2(2)
F(32)-C(32)-C(31)	120.0(2)
C(33)-C(32)-C(31)	118.8(2)
F(33)-C(33)-C(32)	119.4(2)
F(33)-C(33)-C(34)	120.0(2)
C(32)-C(33)-C(34)	120.6(2)
F(34)-C(34)-C(33)	114.67(18)
F(34)-C(34)-C(29)	121.70(19)
C(33)-C(34)-C(29)	123.6(2)
C(40)-C(35)-C(36)	113.19(18)
C(40)-C(35)-B	127.34(17)
C(36)-C(35)-B	119.23(17)
F(36)-C(36)-C(37)	116.28(18)
F(36)-C(36)-C(35)	119.41(18)
C(37)-C(36)-C(35)	124.3(2)
F(37)-C(37)-C(38)	119.69(19)

F(37)-C(37)-C(36)	120.7(2)
C(38)-C(37)-C(36)	119.63(19)
F(38)-C(38)-C(39)	120.5(2)
F(38)-C(38)-C(37)	120.7(2)
C(39)-C(38)-C(37)	118.74(19)
F(39)-C(39)-C(38)	119.67(19)
F(39)-C(39)-C(40)	120.47(19)
C(38)-C(39)-C(40)	119.9(2)
F(40)-C(40)-C(39)	114.91(18)
F(40)-C(40)-C(35)	120.85(17)
C(39)-C(40)-C(35)	124.23(19)
C(42)-C(41)-C(46)	112.89(18)
C(42)-C(41)-B	127.18(18)
C(46)-C(41)-B	119.60(17)
F(42)-C(42)-C(43)	114.92(17)
F(42)-C(42)-C(41)	120.67(18)
C(43)-C(42)-C(41)	124.41(19)
F(43)-C(43)-C(44)	120.07(19)
F(43)-C(43)-C(42)	120.36(19)
C(44)-C(43)-C(42)	119.57(19)
F(44)-C(44)-C(43)	120.5(2)
F(44)-C(44)-C(45)	120.3(2)
C(43)-C(44)-C(45)	119.16(19)
F(45)-C(45)-C(46)	121.49(19)
F(45)-C(45)-C(44)	119.43(19)
C(46)-C(45)-C(44)	119.08(19)
F(46)-C(46)-C(45)	116.20(18)
F(46)-C(46)-C(41)	118.97(17)
C(45)-C(46)-C(41)	124.83(18)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
In	21(1)	27(1)	29(1)	0(1)	-1(1)	-1(1)
F(24)	33(1)	32(1)	31(1)	2(1)	7(1)	9(1)
F(25)	45(1)	53(1)	37(1)	-5(1)	20(1)	9(1)
F(26)	53(1)	60(1)	26(1)	8(1)	14(1)	-6(1)
F(27)	55(1)	41(1)	37(1)	16(1)	3(1)	2(1)
F(28)	35(1)	32(1)	36(1)	5(1)	5(1)	9(1)
F(30)	32(1)	31(1)	28(1)	-5(1)	2(1)	4(1)
F(31)	51(1)	54(1)	25(1)	-7(1)	-2(1)	-17(1)
F(32)	33(1)	87(1)	41(1)	13(1)	-16(1)	-14(1)
F(33)	24(1)	58(1)	74(1)	16(1)	0(1)	11(1)
F(34)	33(1)	34(1)	52(1)	-5(1)	5(1)	10(1)
F(36)	39(1)	38(1)	36(1)	-1(1)	15(1)	-8(1)
F(37)	56(1)	60(1)	31(1)	-7(1)	22(1)	1(1)
F(38)	59(1)	48(1)	32(1)	-18(1)	2(1)	9(1)
F(39)	51(1)	35(1)	46(1)	-14(1)	2(1)	-11(1)
F(40)	34(1)	35(1)	34(1)	-7(1)	11(1)	-11(1)
F(42)	29(1)	36(1)	34(1)	8(1)	-5(1)	-10(1)
F(43)	57(1)	29(1)	36(1)	9(1)	-1(1)	-7(1)
F(44)	51(1)	44(1)	30(1)	9(1)	-2(1)	19(1)
F(45)	26(1)	66(1)	38(1)	5(1)	-7(1)	5(1)
F(46)	25(1)	37(1)	33(1)	1(1)	1(1)	-7(1)
N(1)	24(1)	30(1)	24(1)	1(1)	1(1)	-2(1)
N(2)	26(1)	43(1)	25(1)	7(1)	2(1)	-5(1)
N(3)	26(1)	26(1)	37(1)	-3(1)	-1(1)	0(1)
B	20(1)	23(1)	21(1)	1(1)	3(1)	1(1)
C(1)	28(1)	29(1)	76(2)	-12(1)	-4(1)	-2(1)
C(2)	33(1)	37(1)	25(1)	4(1)	4(1)	0(1)
C(3)	48(2)	75(2)	23(1)	5(1)	1(1)	18(1)
C(4)	47(2)	60(2)	34(1)	-1(1)	8(1)	15(1)
C(5)	27(1)	24(1)	27(1)	3(1)	2(1)	-1(1)
C(6)	32(1)	50(1)	32(1)	2(1)	4(1)	-12(1)

C(7)	32(1)	51(2)	49(2)	8(1)	0(1)	-16(1)
C(8)	41(1)	39(1)	46(1)	9(1)	-13(1)	-17(1)
C(9)	51(2)	46(1)	31(1)	3(1)	-11(1)	-10(1)
C(10)	40(1)	49(1)	27(1)	5(1)	-2(1)	-6(1)
C(11)	26(1)	31(1)	27(1)	5(1)	0(1)	2(1)
C(12)	38(1)	81(2)	32(1)	23(1)	3(1)	-11(1)
C(13)	78(4)	73(4)	50(3)	12(3)	11(3)	-18(4)
C(14)	77(4)	71(4)	42(4)	42(3)	14(3)	-29(3)
C(13A)	50(3)	102(5)	23(2)	13(3)	4(2)	8(3)
C(14A)	140(7)	87(5)	30(4)	32(4)	-5(4)	-62(5)
C(15)	36(1)	35(1)	52(2)	-3(1)	14(1)	-3(1)
C(16)	33(1)	34(1)	55(2)	-5(1)	-15(1)	6(1)
C(17)	28(1)	25(1)	39(1)	-7(1)	7(1)	0(1)
C(18)	33(1)	30(1)	54(2)	-9(1)	2(1)	2(1)
C(19)	36(1)	42(1)	84(2)	-25(1)	10(1)	-6(1)
C(20)	70(2)	35(1)	78(2)	-13(1)	41(2)	-18(1)
C(21)	91(2)	36(1)	49(2)	-1(1)	25(2)	-7(1)
C(22)	55(2)	33(1)	39(1)	-3(1)	8(1)	1(1)
C(23)	20(1)	25(1)	20(1)	-2(1)	0(1)	-4(1)
C(24)	24(1)	26(1)	23(1)	-1(1)	1(1)	-1(1)
C(25)	24(1)	38(1)	25(1)	-7(1)	5(1)	-2(1)
C(26)	33(1)	41(1)	18(1)	0(1)	4(1)	-10(1)
C(27)	34(1)	31(1)	25(1)	7(1)	-4(1)	-5(1)
C(28)	23(1)	27(1)	27(1)	-2(1)	1(1)	-1(1)
C(29)	21(1)	26(1)	23(1)	5(1)	4(1)	-1(1)
C(30)	25(1)	28(1)	21(1)	5(1)	2(1)	-1(1)
C(31)	35(1)	37(1)	19(1)	4(1)	0(1)	-10(1)
C(32)	24(1)	55(1)	30(1)	16(1)	-7(1)	-11(1)
C(33)	20(1)	41(1)	41(1)	14(1)	2(1)	5(1)
C(34)	25(1)	29(1)	32(1)	5(1)	4(1)	0(1)
C(35)	24(1)	25(1)	23(1)	0(1)	2(1)	3(1)
C(36)	29(1)	30(1)	26(1)	1(1)	4(1)	1(1)
C(37)	34(1)	44(1)	23(1)	0(1)	9(1)	7(1)
C(38)	40(1)	35(1)	24(1)	-10(1)	-1(1)	9(1)
C(39)	35(1)	27(1)	30(1)	-4(1)	-3(1)	0(1)
C(40)	27(1)	30(1)	24(1)	-1(1)	3(1)	2(1)

C(41)	23(1)	26(1)	19(1)	-2(1)	3(1)	3(1)
C(42)	26(1)	29(1)	21(1)	-2(1)	0(1)	-1(1)
C(43)	38(1)	25(1)	23(1)	1(1)	5(1)	0(1)
C(44)	38(1)	34(1)	20(1)	2(1)	2(1)	13(1)
C(45)	23(1)	42(1)	22(1)	-3(1)	0(1)	7(1)
C(46)	24(1)	29(1)	22(1)	-3(1)	4(1)	-1(1)

Table 4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 10.

	x	y	z	U(eq)
H(1A)	12082	2028	7877	67
H(1B)	11405	2060	8631	67
H(1C)	11033	2486	7905	67
H(2)	8037	486	8805	38
H(3A)	9950	387	9080	73
H(3B)	9352	668	9796	73
H(3C)	10022	1134	9269	73
H(4A)	8388	1821	9068	70
H(4B)	7652	1363	9561	70
H(4C)	7264	1533	8700	70
H(6)	6812	664	8029	46
H(7)	5530	239	7297	53
H(8)	5543	-51	6086	51
H(9)	6860	154	5308	52
H(10)	8362	700	5508	46
H(12B)	9207(5)	1549(3)	5495(4)	60
H(12A)	9983(4)	1196(3)	5356(3)	60
H(13A)	9167	2317	6037	100
H(13B)	8336	1849	5572	100
H(13C)	9314	2186	5152	100
H(14A)	11086	2071	5619	94
H(14B)	11485	1529	6214	94
H(14C)	10731	2104	6482	94
H(13D)	10495	987	4916	87
H(13E)	10030	473	5487	87
H(13F)	11179	818	5693	87
H(14D)	10305	2341	6154	129
H(14E)	10833	2114	5385	129
H(14F)	11316	1852	6191	129
H(15A)	12833	95	7221	61

H(15B)	12576	834	7056	61
H(15C)	11780	294	6689	61
H(16A)	11910	637	8941	61
H(16B)	12675	1023	8390	61
H(16C)	12898	280	8554	61
H(18)	10002	-52	6958	47
H(19)	8969	-981	7109	64
H(20)	9384	-1658	8137	72
H(21)	10869	-1433	8979	69
H(22)	11866	-492	8859	51
