EXPERIMENTAL

General

An MBraun UL-99-245 dry box and standard Schlenk techniques on a double manifold vacuum line were used in the manipulation of air and moisture sensitive compounds. Anhydrous solvents were used as received from Aldrich Chemical Company. NMR spectra were recorded on a Bruker AC 250 spectrometer in five millimeter quartz tubes at the Atlantic Region Magnetic Resonance Center. ^{1}H and $^{13}C\{^{1}H\}$ chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are calibrated to the residual signal of the solvent. The ^{27}Al NMR were obtained on a Bruker AMX 400 spectrometer in a 10 mm tube with $[Al(H_2O)_6]^{3+}$ as external reference. Infrared spectra were obtained using a Perkin-Elmer Model 683 spectrometer with the % transmittance values reported in cm^{-1}. Melting points were measured using a Mel-Temp apparatus and are uncorrected. Elemental analyses were performed by Atlantic Microlab (Norcross, Ga). Electron impact mass spectral data were obtained at Simon Fraser University (Burnaby, B.C.) using an HP 5985 GC mass spectrometer.

***N,N'*-diisopropyl-2,4,6-triphenylbenzamidine (2H):** To a suspension of 15.0 g (38.9 mmol) of 2,4,6-triphenylbromobenzene in 60 ml anhydrous diethylether and 10 ml anhydrous hexane, 25.0 ml (40.0 mmol) of 1.6 M butyllithium was added drop-wise, and stirred for 4 h at room temperature. *N,N'*-diisopropylcarbodiimide (5.0 g, 39.6 mmol) dissolved in *ca* 15 ml of THF was added drop-wise to the reaction mixture and stirred overnight. After quenching with water, the reaction mixture was transferred to a

separatory funnel and extracted with CH_2Cl_2. The organic layer was washed with water and saturated NaCl and dried over anhydrous magnesium sulfate. After removal of solvent, the yellow solid was dissolved in warm toluene and filtered to remove insoluble white LiBr. Upon cooling, the filtrate formed well-defined crystals that were characterized as *N,N'*-diisopropyl-2,4,6-triphenylbenzamidine (8.14 g, 18.8 mmol, 48%), m.p. 159-160°C. Anal. Calcd for $C_{31}H_{32}N_2$: C, 86.07; H, 7.46; N, 6.48. Found: C, 86.09; H, 7.51; N, 6.45. ^{1}H NMR (CD_2Cl_2): δ = 7.66-7.27 (m, 17H), 3.77 (broad, 1H), 3.43 (broad, 1H), 3.14 (broad, 1H), 1.03 (broad , 6H), 0.55 (broad, 6H). $^{13}C\{^1H\}$NMR (CD_2Cl_2): δ = 152.0, 142.9, 142.2, 141.8, 141.7, 140.8, 133.3, 129.7, 128.6, 128.5, 128.3, 128.2, 128.0, 127.9, 127.7, 25.0, 22.6. IR (Nujol, cm^{-1}): 3420s, 3080w, 3040s, 3020m, 1620s, 1590s, 1490s, 1480s, 1445s, 1310m, 260m, 1180m, 890m, 770s, 725m, 700s. LRMS m/z: 432 (M^+) (13), 374(21), 355(100) 332(92), 58 (26), 43 (47).

***N,N'*-Dicyclohexyl-2,4,6-triphenylbenzamidine (3H):** The synthesis of **3H** followed the procedure given for the synthesis of **2H.** 4.50 g (21.8 mmol) of *N,N'*-dicyclohexylcarbodiimide yielded 5.85 g (11.4 mmol 50%) of **3H**. m.p. 189-190°C. Anal. Calcd for $C_{37}H_{40}N_2$: C, 86.67; H, 7.86; N, 5.46. Found: C, 86.33; H, 8.02; N, 5.34. ^{1}H NMR (CD_2Cl_2): δ = 7.80-7.26 (m, 17H), 3.12 (broad, 1H), 2.85 (broad, 1H), 2.37 (s, 1H), 1.85-0.13 (m, 19H). $^{13}C\{^1H\}$NMR (CD_2Cl_2): δ = 142.5, 140.9, 140.6, 138.5, 136.9, 133.8, 129.5, 129.4, 129.3, 128.7, 128.2, 128.0, 127.8, 127.5, 127.0, 125.8, 125.6, 36.9, 36.6, 35.1, 34.3, 33.8, 32.4, 31.9, 26.9, 26.7, 26.1, 26.0, 25.9, 25.8, 25.6, 21.7. IR (Nujol, cm^{-1}): 3400s, 3080m, 3060m, 1620s, 1590s, 1300m, 1280w, 1250m, 890m, 775w, 760m,

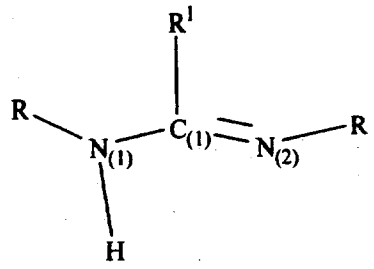
700s. LRMS m/z: 513 (M+1) (5), 512 (M^+) (7), 429 (74), 347(88), 332(99), 330 (48), 317 (32), 98 (50), 83 (21), 67 (18), 56 (28), 55 (100), 42 (15).

X-ray Crystallographic Structural Determination

X: A single crystal of **X** (**X** = **2H, 3H, 2AlMe$_2$,** or **3AlMe$_2$**) was mounted on a Rigaku AFC5R diffractometer equipped with a rotating anode generator and utilizing graphite monochromated Cu-K_α radiation (**2H, 2AlMe$_2$, 3AlMe$_2$**) or Mo-K_α radiation (**3H**). Cell constants and an orientation matrix for data collection were obtained from a least squares refinement using the setting angles of 25 carefully centered reflections. Data were collected at room temperature (23 °C) and were corrected for Lorentz and polarization effects. The structure was solved by direct methods[i] and expanded using Fourier techniques.[ii] Full matrix least squares refinement was carried out using SHELXL97.[iii] The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in their geometrically calculated positions and allowed to ride on the heavy atoms to which they were bonded, with U_{iso} equal to $1.2U_{eq}$ of the heavy atom ($1.5U_{eq}$ for methyl hydrogens). Full details of the structures and the refinements are given in Table 1.

Table 1. Crystal data and structure refinement for Compounds 2H, 3H, $2AlMe_2$, and $3AlMe_2$.

Compound	2H	3H	$2AlMe_2$	$3AlMe_2$
Empirical formula	$C_{31}H_{32}N_2$	$C_{37}H_{40}N_2$	$C_{16.50}H_{18.50}Al_{0.50}N_1$	$C_{39}H_{45}Al_1N_2$
Formula weight (g/mol)	432.61	512.71	244.33	568.78
Temperature (K)	293(2)	293(2)	293(2)	293(2)
Wavelength (Å)	1.5418	0.71069	1.5418	1.5418
Crystal system	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P\ 2_1/n$	*Pbcn*	$P2_1/c$
Unit cell dimensions (Å)	a = 10.979(2)	a = 12.089(4)	a = 14.115(3)	a= 13.619(2)
	b = 28.248(2)	b = 16.871(5)	b = 15.515(3)	b = 12.291(2)
	c = 8.229(2)	c = 14.998(3)	c = 13.377(3)	c = 20.958(2)
(°)	α = 90	α = 90	α = 90	α = 90
(°)	β = 90	β = 103.51(2)	β = 90	β = 102. 002(8)
(°)	γ= 90	γ= 90	γ= 90	γ= 90
Volume ($Å^3$)	2552.2(7)	2975(2)	2929.5(9)	3431.3(7)
Z	4	4	8	4
Density (calculated) Mg/m^3	1.126	1.145	1.108	1.101
Absorption coefficient mm^{-1}	0.495	0.066	0.759	0.712
F(000)	928	1104	1048	1224
Crystal size (mm^3)	0.50 x 0.50 x 0.30	1.00 x 0.75 x 0.45	0.75 x 0.75 x 0.70	0.55 x 0.40 x 0.15
Theta range for data Collection (°)	3.13 to 63.56	2.74 to 30.00	2.85 to 63.53	3.32 to 63.59
Index ranges	0<=h<=12 0<=k<=32 0<=l<= 9	0<=h<=17 0<=k<=23 -20<=l<=20	0<=h<=16 0<=k<=18 0<=l<=15	0<=h<=13, 0<=k<=14 -24<=l<=23
Reflections collected	2417	9239	2720	5759
Independent reflections	2391	8582 [R(int) = 0.0850]	2385	5218 [R(int) = 0.1368]
Absorption correction	Psi scan	Psi scan	Psi scan	None
Max and min. transmission	1.000 and 0.939	1.000 and 0.931	1.000 and 0.787	1.000 and 0.887
Refinement method	Full-matrix least squares on F^2	Full-matrix least squares on F^2	Full-matrix least squares on F^2	Full-matrix least squares on F^2
Data / restraints / parameters	2391 / 0 / 299	8582 / 0 / 353	2385 / 0 / 168	5218 / 0 / 332
Goodness-of-fit on F^2	0.997	0.950	0.953	0.908
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR^2 = 0.0841	R1 = 0.0526, wR^2 = 0.1416	R1 = 0.0372, wR^2 = 0.0953	R1 = 0.0453, wR2 = 0.0968
R indices (all data)	R1 = 0.0916, wR^2 = 0.1050	R1 = 0.2971, wR^2 = 0.2327	R1 =0.2065, wR^2 = 0.1401	R1 = 0.3687, wR2 = 0.1813
Extinction coefficient	0.0057(4)	0.0038(10)	0.0049(3)	0.00107(11)



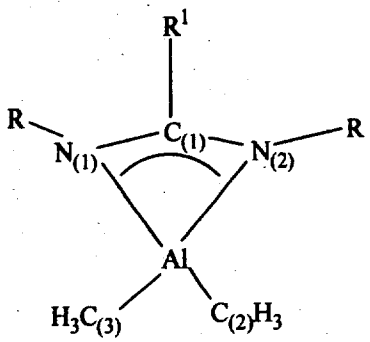


Chart 1

Table 2. Selected bond lengths and bond angles of amidines and corresponding amidinates

Selected bond lengths [Å]	2H	3H	$2AlMe_2$	$3AlMe_2$	$tBu\text{-}C\{(N\text{-}Cy)_2AlMe_2$ Error! Bookmark not defined.
N(1)-C(1)	1.368(4)	1.379(4)	1.325(3)	1.325(7)	1.343(2)
N(2)-C(1)	1.282(4)	1.283(3)	1.325(3)	1.328(7)	1.339(2)
C(1)-R^1	1.513(4)	1.498(4)	1.506(5)	1.508(7)	1.540(2)
N(1)-R	1.462(4)	1.450(4)	1.465(4)	1.447(7)	1.456(2)
N(2)-R	1.460(4)	1.462(4)	1.465(4)	1.458(7)	1.454(2)
Al-C(3)			1.947(3)	1.949(7)	-
Al-N(1)			1.917(3)	1.936(5)	-
Al-C(2)			1.947(3)	1.944(7)	1.958(2)
Al-N(2)			1.917(3)	1.942(5)	1.9124(14)
Selected bond angles [°]					
N(1)-C(1)-N(2)	120.2(3)	119.8(3)	109.3(4)	110.8(6)	107.8
R^1-C(1)-N(1)	113.4(3)	114.0(2)	125.4(2)	124.2(6)	-
R^1-C(1)-N(2)	126.4(3)	126.2(3)	125.4(2)	125.0(6)	-
C(1)-N(1)-R	122.5(3)	122.9(2)	127.8(3)	126.6(6)	131.4
C(1)-N(1)-H or Al	121.8	118.6	91.1(2)	90.5(4)	91.3
R-N(1)-H or Al	112.2	118.6	141.2(2)	142.8(4)	136.5
C(1)-N(2)-R	120.7(3)	120.5(2)	127.8(3)	126.0(5)	132.5
C(1)-N(2)-Al			91.1(2)	90.1(4)	92.1
R-N(2)-Al			141.2(2)	143.8(4)	133.4
N(1)-Al-N(2)			68.6(2)	68.5(2)	68.7
N(1)-Al-C(3)			115.32(13)	114.8(3)	-
N(2)-Al-C(2)			115.32(13)	115.6(3)	-
C(3)-Al-C(2)			117.4(2)	119.2(3)	116.2

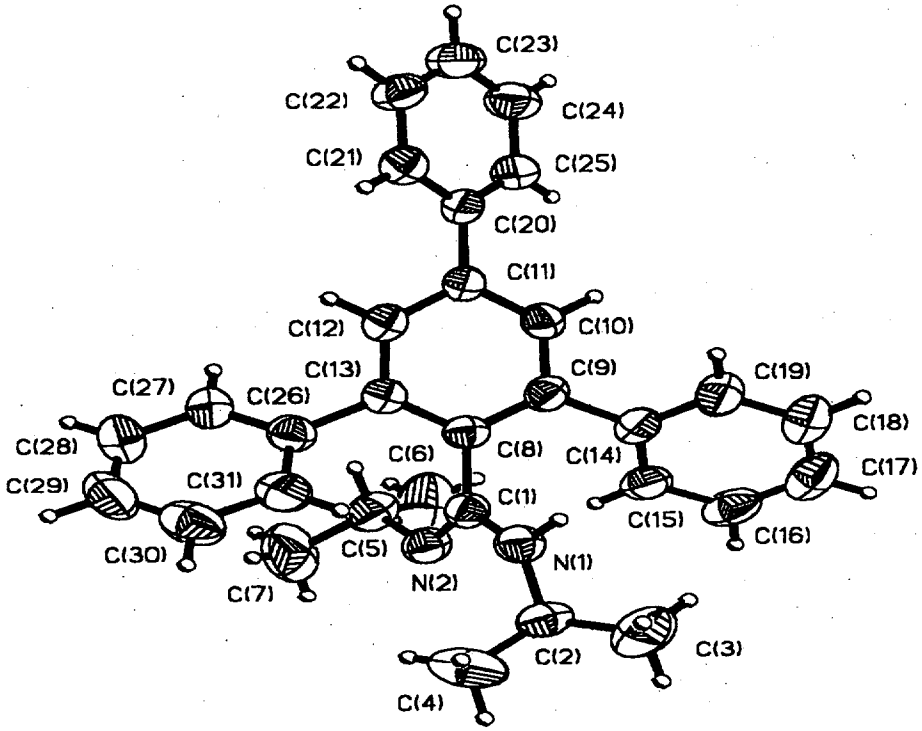


Figure S1 – ORTEP view of the molecular structure of 2H showing the labeling scheme. Thermal ellipsoids are shown at 50% probability level; hydrogen atoms, except H(1), have been removed for clarity; selected bond lengths [Å]: N(1)-C(1) 1.368(4), N(1)-C(2) 1.462(4), N(1)-H(1) 0.8900, N(2)-C(1) 1.282(4), N(2)-C(5) 1.460(4), C(1)-C(8) 1.513(4); selected bond angles [°]: C(1)-N(1)-C(2) 122.5(3), C(1)-N(1)-H(1)121.8, C(2)-N(1)-H(1) 112.2, C(1)-N(2)-C(5) 120.7(3), N(2)-C(1)-N(1) 120.2(3), N(2)-C(1)-C(8) 126.4(3), N(1)-C(1)-C(8) 113.4(3); selected torsion angle [°] N(1)-C(1)-C(8)-C(9) 70.75(0.39).

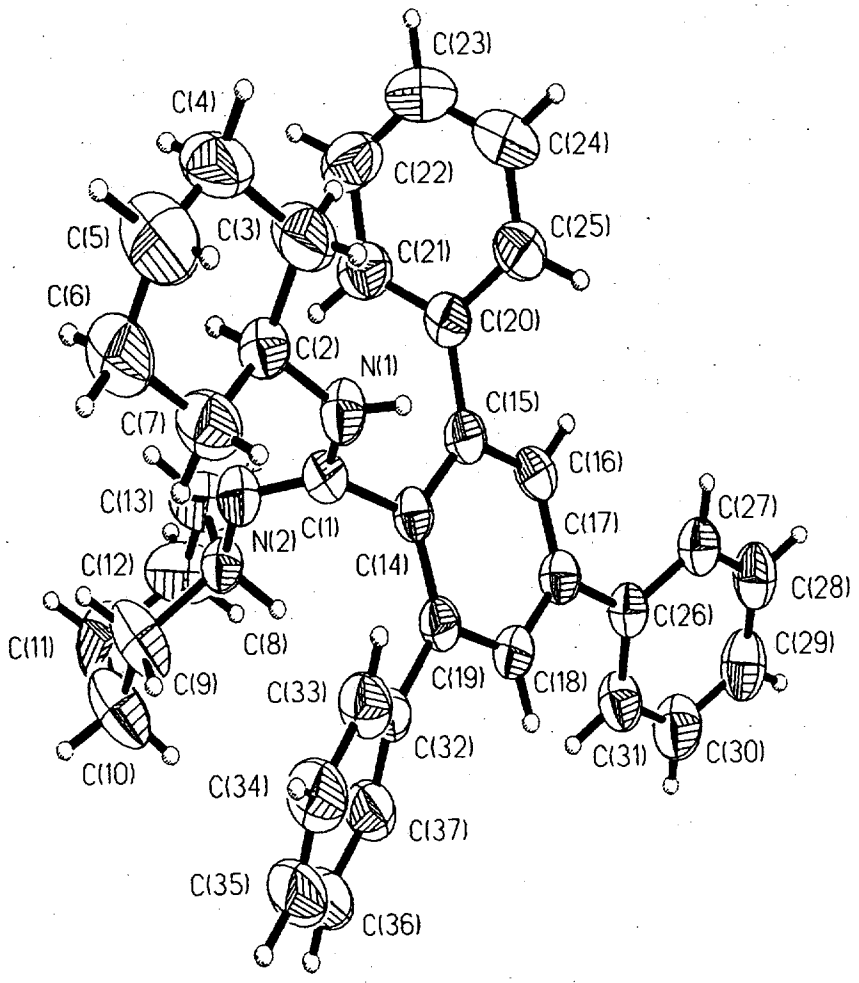


Figure S2 – ORTEP view of the molecular structure of 3H showing the labeling scheme. Thermal ellipsoids are shown at 50% probability level; hydrogen atoms, except H(1), have been removed for clarity; selected bond lengths [Å]: N(1)-C(1) 1.379(4), N(1)-C(2) 1.450(4), N(1)-H(1) 0.8600, N(2)-C(1) 1.283(3), N(2)-C(8) 1.462(4), C(1)-C(14) 1.498(4); selected bond angles [°]: C(1)-N(1)-C(2) 122.9(2), C(1)-N(1)-H(1) 118.6, C(2)-N(1)-H(1) 118.6, C(1)-N(2)-C(8) 120.5(2), N(2)-C(1)-N(1) 119.8(3), N(2)-C(1)-C(14) 126.2(3), N(1)-C(1)-C(14) 114.0(2); selected torsion angle [°] N(1)-C(1)-C(14)-C(15) –70.29(0.34).

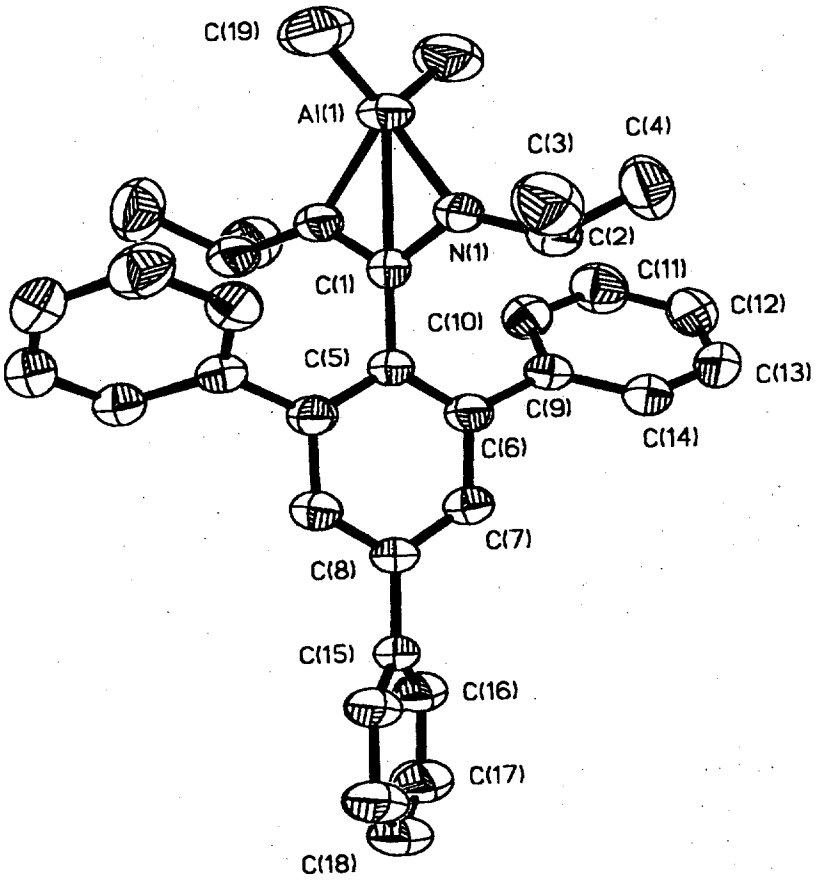


Figure S3 – ORTEP view of the dialkylaluminum amidinate complex, $2AlMe_2$ showing the labeling scheme. Thermal ellipsoids are shown at 50% probability level; hydrogen atoms have been removed for clarity; the symmetry (1-x, y, 0.5-z) is required to generate the second half of the molecule; selected bond lengths [Å]:Al(1)-N(1) 1.917(3), Al(1)-C(19) 1.947(3), Al(1)-C(1) 2.351(4), N(1)-C(1) 1.325(3), N(1)-C(2) 1.465(4), C(1)-C(5) 1.506(5). Selected bond angles [°]: N(1)-Al(1)-N(1A) 68.6(2), C(19)-Al(1)-C(19A) 117.4(2), C(1)-N(1)-C(2) 127.8(3), C(1)-N(1)-Al(1) 91.1(2), C(2)-N(1)-Al(1) 141.2(2) N(1)-C(1)-C(5) 125.4(2); selected torsion angle [°] N(1)-C(1)-C(5)-C(6) -64.24(0.20).

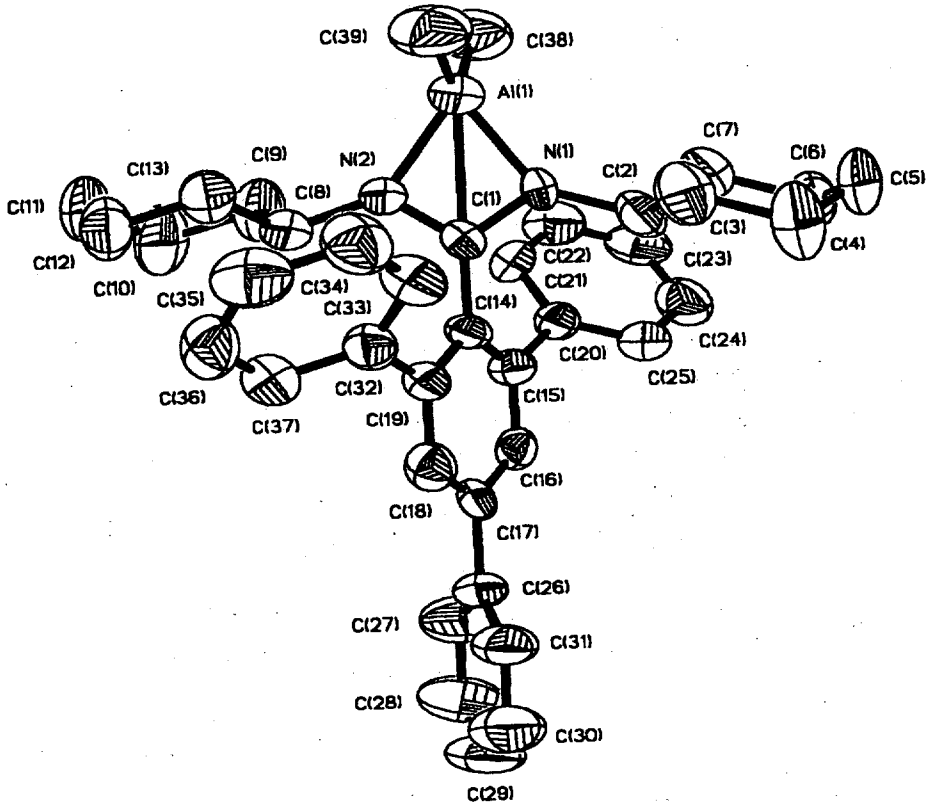


Figure S4 – ORTEP view of the dialkylaluminum amidinate complex $3AlMe_2$, showing the labeling scheme. Thermal ellipsoids are shown at 50% probability level; hydrogen atoms have been removed for clarity; selected bond lengths [Å]:Al(1)-N(1) 1.936(5), Al(1)-N(2) 1.942(5), Al(1)-C(39) 1.944(7), Al(1)-C(38) 1.949(7), Al(1)-C(1) 2.355(7), N(1)-C(1) 1.325(7), N(1)-C(2) 1.447, N(2)-C(8) 1.458(7), N(2)-C(1) 1.328(7), C(1)-C(14) 1.508(7). Selected bond angles [°]: N(1)-Al(1)-N(2) 68.5(2), N(1)-Al(1)-C(39) 114.8(3), C(1)-N(1)-Al(1) 90.5(4), N(1)-C(1)-N(2) 110.8(6), C(1)-N(1)-C(2) 126.6(6), N(1)-C(1)-C(14) 124.2(6); selected torsion angle [°] N(1)-C(1)-C(14)-C(15) –69.95(0.75).

Compound 2H

Table 1. Crystal data and structure refinement.

Identification code	jason42
Empirical formula	C31 H32 N2
Formula weight	432.61
Temperature	293(2)K
Wavelength	1.5418Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 10.979(2)Å alpha = 90°
	b = 28.248(2)Å beta = 90°
	c = 8.229(2)Å gamma = 90°
Volume	2552.2(7)Å^3
Z	4
Density (calculated)	1.126 Mg/m^3
Absorption coefficient	0.495 mm^{-1}
F(000)	928
Crystal size	0.50 x 0.50 x 0.30 mm
Theta range for data collection	3.13° to 63.56°
Index ranges	0<=h<=12, 0<=k<=32, 0<=l<=9
Reflections collected	2417
Independent reflections	2391 [R(int) = 0.0000]
Absorption correction	Psi scan
Max. and min. transmission	1.000 and 0.939
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2391 / 0 / 299
Goodness-of-fit on F^2	0.997
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0841
R indices (all data)	R1 = 0.0916, wR2 = 0.1050
Absolute structure parameter	-0.4(11)
Extinction coefficient	0.0057(4)
Largest diff. peak and hole	0.124 and -0.117 e.Å^{-3}

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

	x	y	z	U(eq)
N(1)	4199(2)	3262(1)	8091(3)	52(1)
N(2)	3239(2)	3421(1)	5671(3)	52(1)
C(1)	3973(3)	3553(1)	6795(4)	46(1)
C(2)	3807(3)	2768(1)	8133(5)	60(1)
C(3)	4719(4)	2485(1)	9110(6)	101(2)
C(4)	2534(4)	2729(2)	8787(6)	94(2)
C(5)	2971(3)	3731(1)	4298(5)	63(1)
C(6)	3707(5)	3591(2)	2822(5)	110(2)
C(7)	1628(4)	3699(2)	3946(7)	117(2)
C(8)	4668(3)	4015(1)	6862(4)	45(1)
C(9)	5940(3)	4015(1)	6614(4)	46(1)
C(10)	6549(3)	4445(1)	6593(4)	47(1)
C(11)	5968(3)	4876(1)	6870(4)	47(1)
C(12)	4725(3)	4860(1)	7177(4)	53(1)
C(13)	4067(3)	4441(1)	7167(4)	45(1)
C(14)	6700(3)	3575(1)	6444(4)	51(1)
C(15)	6358(3)	3181(1)	5541(5)	58(1)
C(16)	7122(4)	2791(1)	5418(5)	70(1)
C(17)	8243(4)	2788(1)	6159(5)	79(1)
C(18)	8594(4)	3174(1)	7057(5)	76(1)
C(19)	7828(3)	3561(1)	7216(5)	62(1)
C(20)	6646(3)	5329(1)	6860(4)	48(1)
C(21)	6273(3)	5711(1)	7825(5)	58(1)
C(22)	6877(4)	6137(1)	7769(5)	66(1)
C(23)	7880(4)	6195(1)	6794(5)	69(1)
C(24)	8281(4)	5823(1)	5855(5)	65(1)

C(25)	7657(3)	5396(1)	5885(4)	53(1)
C(26)	2720(3)	4474(1)	7473(4)	52(1)
C(27)	2062(3)	4825(1)	6703(5)	67(1)
C(28)	826(4)	4880(2)	7004(6)	83(1)
C(29)	246(3)	4595(2)	8097(6)	83(1)
C(30)	890(4)	4244(2)	8856(6)	77(1)
C(31)	2118(3)	4184(1)	8560(4)	60(1)

Table 3A. Bond lengths [Å].

N(1)-C(1)	1.368(4)
N(1)-C(2)	1.462(4)
N(1)-H(1)	0.8900
N(2)-C(1)	1.282(4)
N(2)-C(5)	1.460(4)
C(1)-C(8)	1.513(4)
C(2)-C(4)	1.502(5)
C(2)-C(3)	1.513(5)
C(2)-H(2)	0.9800
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-C(7)	1.506(5)
C(5)-C(6)	1.511(6)
C(5)-H(5)	0.9800
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-C(13)	1.395(4)
C(8)-C(9)	1.412(4)
C(9)-C(10)	1.388(4)
C(9)-C(14)	1.503(4)
C(10)-C(11)	1.393(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.389(4)
C(11)-C(20)	1.480(4)
C(12)-C(13)	1.387(4)
C(12)-H(12)	0.9300

C(13)-C(26)	1.503(4)
C(14)-C(15)	1.390(4)
C(14)-C(19)	1.392(5)
C(15)-C(16)	1.388(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.374(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.373(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.386(4)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(25)	1.383(4)
C(20)-C(21)	1.399(4)
C(21)-C(22)	1.376(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.373(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.378(5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.386(4)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-C(27)	1.379(5)
C(26)-C(31)	1.383(5)
C(27)-C(28)	1.389(5)
C(27)-H(27)	0.9300
C(28)-C(29)	1.365(6)
C(28)-H(28)	0.9300
C(29)-C(30)	1.369(6)
C(29)-H(29)	0.9300
C(30)-C(31)	1.380(5)
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300

Table 3B. Bond angles [°].

C(1)-N(1)-C(2)	122.5(3)
C(1)-N(1)-H(1)	121.8
C(2)-N(1)-H(1)	112.2
C(1)-N(2)-C(5)	120.7(3)
N(2)-C(1)-N(1)	120.2(3)
N(2)-C(1)-C(8)	126.4(3)
N(1)-C(1)-C(8)	113.4(3)
N(1)-C(2)-C(4)	110.7(3)
N(1)-C(2)-C(3)	108.9(3)
C(4)-C(2)-C(3)	112.7(4)
N(1)-C(2)-H(2)	108.1
C(4)-C(2)-H(2)	108.1
C(3)-C(2)-H(2)	108.1
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(2)-C(5)-C(7)	108.0(3)
N(2)-C(5)-C(6)	111.0(3)
C(7)-C(5)-C(6)	110.7(4)
N(2)-C(5)-H(5)	109.0
C(7)-C(5)-H(5)	109.0
C(6)-C(5)-H(5)	109.0
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5

C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(13)-C(8)-C(9)	119.6(3)
C(13)-C(8)-C(1)	120.8(3)
C(9)-C(8)-C(1)	119.6(3)
C(10)-C(9)-C(8)	118.5(3)
C(10)-C(9)-C(14)	117.1(3)
C(8)-C(9)-C(14)	124.3(3)
C(9)-C(10)-C(11)	122.9(3)
C(9)-C(10)-H(10)	118.5
C(11)-C(10)-H(10)	118.5
C(12)-C(11)-C(10)	116.8(3)
C(12)-C(11)-C(20)	121.6(3)
C(10)-C(11)-C(20)	121.6(3)
C(13)-C(12)-C(11)	122.7(3)
C(13)-C(12)-H(12)	118.7
C(11)-C(12)-H(12)	118.7
C(12)-C(13)-C(8)	119.4(3)
C(12)-C(13)-C(26)	117.2(3)
C(8)-C(13)-C(26)	123.4(3)
C(15)-C(14)-C(19)	117.5(3)
C(15)-C(14)-C(9)	124.2(3)
C(19)-C(14)-C(9)	118.3(3)
C(16)-C(15)-C(14)	120.8(4)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	120.9(4)
C(17)-C(16)-H(16)	119.5
C(15)-C(16)-H(16)	119.5
C(18)-C(17)-C(16)	119.1(4)
C(18)-C(17)-H(17)	120.5

C(16)-C(17)-H(17)	120.5
C(17)-C(18)-C(19)	120.5(4)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	121.2(4)
C(18)-C(19)-H(19)	119.4
C(14)-C(19)-H(19)	119.4
C(25)-C(20)-C(21)	117.4(3)
C(25)-C(20)-C(11)	121.6(3)
C(21)-C(20)-C(11)	121.0(3)
C(22)-C(21)-C(20)	121.0(4)
C(22)-C(21)-H(21)	119.5
C(20)-C(21)-H(21)	119.5
C(23)-C(22)-C(21)	120.7(4)
C(23)-C(22)-H(22)	119.7
C(21)-C(22)-H(22)	119.7
C(22)-C(23)-C(24)	119.5(3)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(23)-C(24)-C(25)	119.8(4)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(20)-C(25)-C(24)	121.7(3)
C(20)-C(25)-H(25)	119.2
C(24)-C(25)-H(25)	119.2
C(27)-C(26)-C(31)	118.2(3)
C(27)-C(26)-C(13)	118.9(3)
C(31)-C(26)-C(13)	122.8(3)
C(26)-C(27)-C(28)	120.7(4)
C(26)-C(27)-H(27)	119.6
C(28)-C(27)-H(27)	119.6
C(29)-C(28)-C(27)	120.4(4)
C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8
C(28)-C(29)-C(30)	119.2(4)
C(28)-C(29)-H(29)	120.4

Table 3B. Bond angles [°] continued.

C(30)-C(29)-H(29)	120.4
C(29)-C(30)-C(31)	120.8(4)
C(29)-C(30)-H(30)	119.6
C(31)-C(30)-H(30)	119.6
C(30)-C(31)-C(26)	120.6(4)
C(30)-C(31)-H(31)	119.7
C(26)-C(31)-H(31)	119.7

Table 3C. Selected torsion angles [°].

178.76	(0.29)	C5 - N2 - C1 - N1
-1.78	(0.47)	C5 - N2 - C1 - C8
10.96	(0.46)	C2 - N1 - C1 - N2
-168.56	(0.28)	C2 - N1 - C1 - C8
-87.43	(0.42)	C1 - N1 - C2 - C4
148.14	(0.34)	C1 - N1 - C2 - C3
-138.68	(0.37)	C1 - N2 - C5 - C7
99.85	(0.40)	C1 - N2 - C5 - C6
71.36	(0.45)	N2 - C1 - C8 - C13
-109.15	(0.34)	N1 - C1 - C8 - C13
-108.74	(0.38)	N2 - C1 - C8 - C9
70.75	(0.39)	N1 - C1 - C8 - C9
-3.55	(0.48)	C13 - C8 - C9 - C10
176.54	(0.31)	C1 - C8 - C9 - C10
173.54	(0.31)	C13 - C8 - C9 - C14
-6.36	(0.51)	C1 - C8 - C9 - C14
2.69	(0.50)	C8 - C9 - C10 - C11
-174.61	(0.33)	C14 - C9 - C10 - C11
-0.04	(0.53)	C9 - C10 - C11 - C12
179.22	(0.31)	C9 - C10 - C11 - C20
-1.82	(0.56)	C10 - C11 - C12 - C13
178.92	(0.33)	C20 - C11 - C12 - C13

0.93	(0.54)	C11 - C12 - C13 - C8
-178.35	(0.33)	C11 - C12 - C13 - C26
1.83	(0.48)	C9 - C8 - C13 - C12
-178.27	(0.33)	C1 - C8 - C13 - C12
-178.94	(0.31)	C9 - C8 - C13 - C26
0.96	(0.48)	C1 - C8 - C13 - C26
-140.59	(0.34)	C10 - C9 - C14 - C15
42.28	(0.52)	C8 - C9 - C14 - C15
38.37	(0.45)	C10 - C9 - C14 - C19
-138.76	(0.34)	C8 - C9 - C14 - C19
-0.18	(0.52)	C19 - C14 - C15 - C16
178.78	(0.33)	C9 - C14 - C15 - C16
-1.25	(0.60)	C14 - C15 - C16 - C17
1.28	(0.61)	C15 - C16 - C17 - C18
0.12	(0.60)	C16 - C17 - C18 - C19
-1.58	(0.59)	C17 - C18 - C19 - C14
1.58	(0.52)	C15 - C14 - C19 - C18
-177.44	(0.33)	C9 - C14 - C19 - C18
-149.40	(0.34)	C12 - C11 - C20 - C25
31.38	(0.49)	C10 - C11 - C20 - C25
29.63	(0.51)	C12 - C11 - C20 - C21
-149.59	(0.33)	C10 - C11 - C20 - C21
1.50	(0.50)	C25 - C20 - C21 - C22
-177.57	(0.33)	C11 - C20 - C21 - C22
-1.68	(0.57)	C20 - C21 - C22 - C23
0.42	(0.58)	C21 - C22 - C23 - C24
0.96	(0.57)	C22 - C23 - C24 - C25
-0.11	(0.48)	C21 - C20 - C25 - C24
178.95	(0.32)	C11 - C20 - C25 - C24
-1.11	(0.55)	C23 - C24 - C25 - C20
44.16	(0.47)	C12 - C13 - C26 - C27
-135.09	(0.37)	C8 - C13 - C26 - C27

Table 3C. Selected torsion angles [°].

-132.42 (0.37)	C12 - C13 - C26 - C31
48.33 (0.48)	C8 - C13 - C26 - C31
-0.58 (0.57)	C31 - C26 - C27 - C28
-177.32 (0.37)	C13 - C26 - C27 - C28
1.49 (0.66)	C26 - C27 - C28 - C29
-2.03 (0.65)	C27 - C28 - C29 - C30
1.71 (0.63)	C28 - C29 - C30 - C31
-0.83 (0.60)	C29 - C30 - C31 - C26
0.26 (0.53)	C27 - C26 - C31 - C30
176.86 (0.34)	C13 - C26 - C31 - C30

Table 4. Selected contact distances [Å] and angles [°] and best plane calculations.

Specified potential hydrogen bonds and other contacts (with esds except fixed and riding H)

D-H	H...A	D...A	<(DHA)	
0.93	2.78	3.485(5)	133.6	C31-H31...N1
0.93	2.74	3.493(4)	138.1	C15-H15...N2
0.98	2.57	3.322(5)	133.5	C5-H5...C13
0.98	2.69	3.363(5)	126.2	C5-H5...C26
0.93	3.06	3.671(5)	124.9	C19-H19...C24_$1
0.93	2.98	3.622(5)	127.8	C24-H24...C9_$2
0.93	3.02	3.713(5)	132.3	C25-H25...C11_$2
0.93	3.03	3.917(5)	161.1	C27-H27...C31_$3
0.98	2.58	3.547(6)	170.5	C2-H2...H17_$4
0.96	2.61	3.419(6)	142.1	C6-H6A...H23_$2
0.96	2.60	3.469(6)	150.4	C6-H6B...H31_$5
0.96	2.56	3.294(6)	133.6	C6-H6C...H17_$4
0.93	2.28	2.735(4)	109.7	C10-H10...H25

0.93	2.28	2.650(4)	103.1	C10-H10...H19
0.93	2.26	2.731(5)	110.3	C12-H12...H21
0.93	2.38	2.727(5)	101.6	C12-H12...H27
0.93	2.32	3.088(6)	139.1	C15-H15...H6A
0.93	2.56	3.168(6)	123.0	C21-H21...H7C_$6

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

- 8.9129 (0.0153) x + 8.6647 (0.0640) y + 4.0889 (0.0098) z = 2.3555 (0.0311)

*	0.0370 (0.0020)	N1
*	0.0405 (0.0025)	N2
*	-0.0399 (0.0021)	C1
*	-0.0243 (0.0010)	C2
*	-0.0133 (0.0017)	C5
	-0.6832 (0.0066)	C3
	1.3432 (0.0065)	C4
	-1.3935 (0.0058)	C6
	1.0123 (0.0070)	C7
	-0.2314 (0.0065)	C8

Rms deviation of fitted atoms = 0.0328

1.8462 (0.0146) x - 2.7935 (0.0377) y + 8.0712 (0.0032) z = 5.2945 (0.0189)

Angle to previous plane (with approximate esd) = 71.31 (0.10)

*	-0.0162 (0.0023)	C8
*	0.0189 (0.0023)	C9
*	-0.0063 (0.0024)	C10
*	-0.0097 (0.0026)	C11

```
*     0.0128 (0.0026)  C12
*     0.0004 (0.0023)  C13
     -0.0692 (0.0057)  C1
      0.1452 (0.0055)  C14
     -0.0196 (0.0055)  C20
     -0.0109 (0.0056)  C26

Rms deviation of fitted atoms =   0.0123


 4.5819 (0.0154) x + 11.4175 (0.0385) y - 6.6980 (0.0078) z = 2.8294
(0.0202)

Angle to previous plane (with approximate esd) = 39.82 ( 0.10 )

*     0.0057 (0.0024)  C14
*     0.0041 (0.0026)  C15
*    -0.0093 (0.0029)  C16
*     0.0046 (0.0028)  C17
*     0.0053 (0.0028)  C18
*    -0.0104 (0.0026)  C19
      0.0462 (0.0056)  C9

Rms deviation of fitted atoms =   0.0070


 6.4910 (0.0133) x - 8.7681 (0.0384) y + 6.1258 (0.0084) z = 3.8479
(0.0264)

Angle to previous plane (with approximate esd) = 61.01 ( 0.10 )

*    -0.0048 (0.0022)  C20
*     0.0101 (0.0025)  C21
*    -0.0062 (0.0026)  C22
*    -0.0030 (0.0026)  C23
*     0.0081 (0.0026)  C24
*    -0.0042 (0.0023)  C25
     -0.0411 (0.0054)  C11
```

Rms deviation of fitted atoms = 0.0065

2.3822 (0.0170) x + 17.9395 (0.0358) y + 6.1008 (0.0091) z = 13.2324 (0.0100)

Angle to previous plane (with approximate esd) = 61.12 (0.11)

*	0.0010	(0.0025)	C26
*	0.0032	(0.0029)	C27
*	-0.0082	(0.0031)	C28
*	0.0090	(0.0029)	C29
*	-0.0048	(0.0029)	C30
*	-0.0002	(0.0026)	C31
	0.0751	(0.0057)	C13

Rms deviation of fitted atoms = 0.0055

Symmetry transformations used to generate equivalent atoms:

$1	-x+3/2, -y+1, z+1/2
$2	-x+3/2, -y+1, z-1/2
$3	-x+1/2, -y+1, z-1/2
$4	x-1/2, -y+1/2, -z+1
$5	x, y, z-1
$6	-x+1/2, -y+1, z+1/2

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^3$).
The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

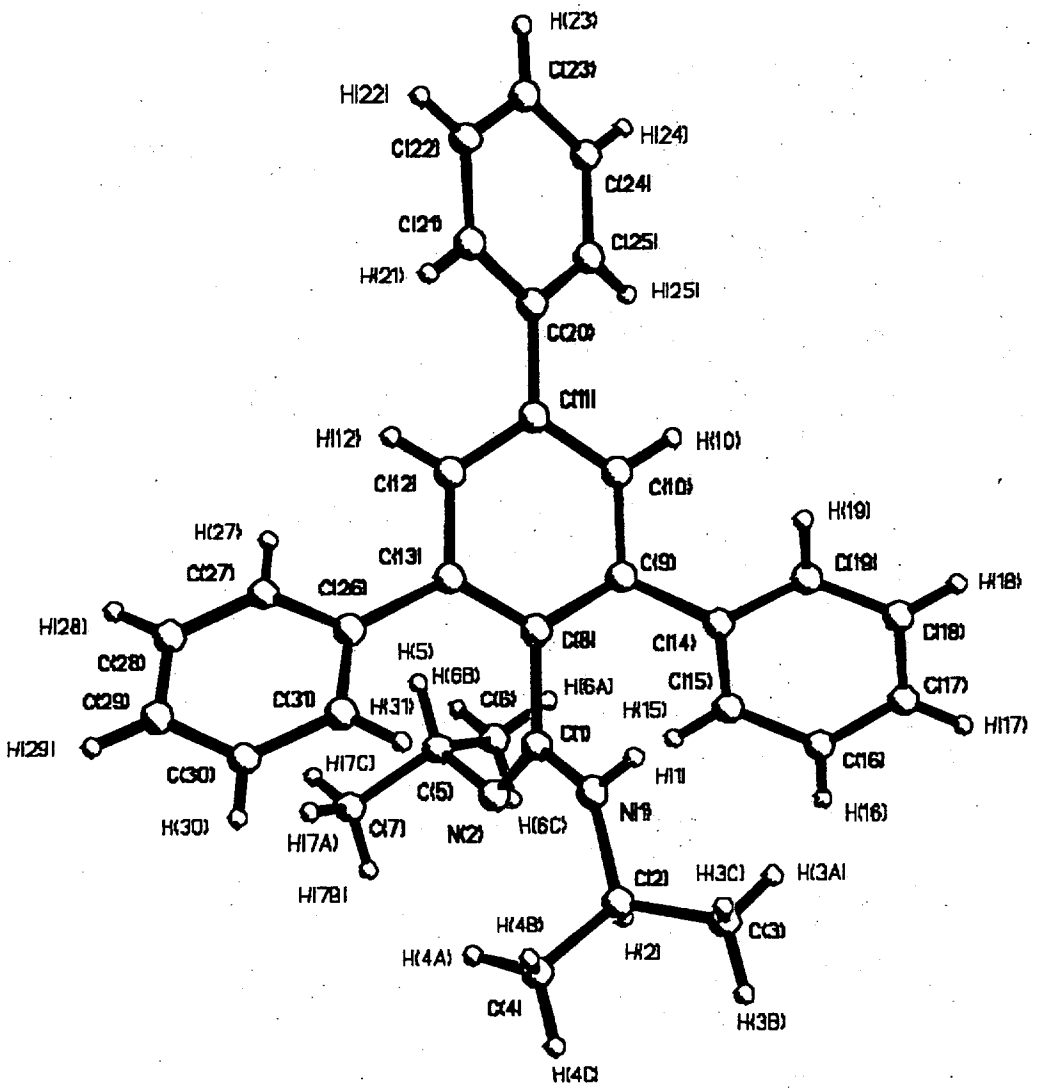
	U11	U22	U33	U23	U13	U12
N(1)	53(2)	53(2)	50(2)	4(1)	-9(2)	-5(1)
N(2)	57(2)	47(2)	53(2)	2(1)	-10(2)	-1(1)
C(1)	46(2)	45(2)	47(2)	2(2)	-1(2)	2(2)
C(2)	71(2)	42(2)	67(2)	8(2)	0(2)	-8(2)
C(3)	114(4)	75(3)	114(4)	35(3)	-20(3)	9(3)
C(4)	90(3)	91(3)	102(4)	-5(3)	18(3)	-38(3)
C(5)	76(3)	54(2)	58(2)	-2(2)	-22(2)	5(2)
C(6)	121(4)	146(5)	63(3)	23(3)	0(3)	44(4)
C(7)	76(3)	149(4)	126(4)	33(4)	-36(3)	19(3)
C(8)	48(2)	43(2)	44(2)	2(2)	-1(2)	-4(1)
C(9)	49(2)	41(2)	48(2)	-2(2)	-1(2)	3(2)
C(10)	40(2)	48(2)	53(2)	-2(2)	3(2)	0(2)
C(11)	43(2)	42(2)	55(2)	-2(2)	-4(2)	4(1)
C(12)	49(2)	45(2)	66(2)	-6(2)	-1(2)	6(2)
C(13)	42(2)	42(2)	51(2)	-2(2)	0(2)	0(2)
C(14)	56(2)	44(2)	52(2)	4(2)	5(2)	7(2)
C(15)	64(2)	43(2)	68(2)	0(2)	7(2)	-2(2)
C(16)	88(3)	42(2)	81(3)	-10(2)	17(2)	5(2)
C(17)	90(3)	59(2)	88(3)	5(2)	14(3)	28(2)
C(18)	75(3)	70(2)	83(3)	7(2)	1(2)	26(2)
C(19)	61(2)	56(2)	70(2)	0(2)	-2(2)	13(2)
C(20)	46(2)	41(2)	56(2)	1(2)	-7(2)	5(1)
C(21)	52(2)	52(2)	71(3)	-10(2)	-5(2)	4(2)
C(22)	73(2)	44(2)	83(3)	-14(2)	-18(2)	2(2)
C(23)	72(3)	51(2)	84(3)	1(2)	-14(3)	-13(2)

C(24)	65(2)	61(2)	71(2)	5(2)	-1(2)	-13(2)
C(25)	53(2)	48(2)	59(2)	-4(2)	-2(2)	-2(2)
C(26)	46(2)	51(2)	58(2)	-9(2)	4(2)	-1(2)
C(27)	50(2)	59(2)	93(3)	5(2)	4(2)	6(2)
C(28)	48(2)	85(3)	115(4)	-4(3)	-4(3)	12(2)
C(29)	42(2)	102(3)	103(3)	-19(3)	6(2)	-2(2)
C(30)	64(3)	88(3)	77(3)	-11(2)	20(2)	-17(2)
C(31)	57(2)	63(2)	60(2)	-9(2)	4(2)	-4(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3).

	x	y	z	U(eq)
H(1)	4804	3319	8784	62
H(2)	3809	2647	7018	72
H(3A)	5515	2522	8646	151
H(3B)	4494	2156	9093	151
H(3C)	4725	2596	10212	151
H(4A)	1992	2914	8128	142
H(4B)	2514	2843	9885	142
H(4C)	2282	2403	8766	142
H(5)	3173	4058	4597	75
H(6A)	4559	3614	3069	165
H(6B)	3515	3800	1936	165
H(6C)	3513	3272	2523	165
H(7A)	1176	3796	4888	175
H(7B)	1421	3378	3677	175
H(7C)	1430	3902	3049	175
H(10)	7382	4446	6384	56
H(12)	4317	5141	7398	64
H(15)	5609	3178	5013	70

H(16)	6871	2528	4826	84
H(17)	8756	2528	6054	95
H(18)	9352	3175	7562	91
H(19)	8072	3816	7851	75
H(21)	5608	5675	8514	70
H(22)	6602	6389	8399	80
H(23)	8287	6484	6768	83
H(24)	8967	5857	5203	79
H(25)	7926	5148	5232	64
H(27)	2451	5026	5974	81
H(28)	390	5113	6457	99
H(29)	-576	4639	8323	99
H(30)	495	4043	9580	92
H(31)	2544	3946	9097	72


H(23)
C(23)
H(22)
H(24)
C(22)
C(24)
C(21)
C(25)
H(21)
H(25)
C(20)
C(11)
H(12)
H(10)
C(12)
C(10)
H(19)
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C(9)
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H(18)
C(27)
C(26)
H(28)
C(8)
C(14)
C(18)
H(5)
C(28)
H(6B)
H(6A)
C(15)
C(17)
C(29)
C(31)
H(31)
C(6)
H(15)
C(1)
H(29)
H(17)
C(30)
H(17C)
H(1)
C(16)
C(5)
N(1)
H(16)
H(30)
H(17A)
C(7)
N(2)
H(6C)
H(17B)
C(2)
H(3C)
H(3A)
H(4B)
C(3)
H(4A)
H(2)
C(4)
H(3B)
H(4C)

Compound 3H

Table 1. Crystal data and structure refinement.

Identification code	jason30
Empirical formula	C37 H40 N2
Formula weight	512.71
Temperature	293(2)K
Wavelength	0.71069Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 12.089(4)Å alpha = 90°
	b = 16.871(5)Å beta = 103.51(2)°
	c = 14.998(3)Å gamma = 90°
Volume	2975(2)Å^3
Z	4
Density (calculated)	1.145 Mg/m^3
Absorption coefficient	0.066 mm^{-1}
F(000)	1104
Crystal size	1.00 x 0.75 x 0.45 mm
Theta range for data collection	2.74° to 30.00°
Index ranges	0<=h<=17, 0<=k<=23, -20<=l<=20
Reflections collected	9239
Independent reflections	8582 [R(int) = 0.08496]
Absorption correction	Psi scan
Max. and min. transmission	1.000 and 0.931
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8582 / 0 / 353
Goodness-of-fit on F^2	0.950
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.1416
R indices (all data)	R1 = 0.2971, wR2 = 0.2327
Extinction coefficient	0.0038(10)
Largest diff. peak and hole	0.261 and -0.290 e.Å^{-3}

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

	x	y	z	U(eq)
N(1)	10897(2)	3712(2)	1855(2)	49(1)
N(2)	10267(2)	2430(1)	1926(2)	46(1)
C(1)	10388(2)	3131(2)	2267(2)	41(1)
C(2)	11438(3)	3549(2)	1107(2)	48(1)
C(3)	12392(3)	4121(3)	1113(3)	78(1)
C(4)	12974(3)	3935(3)	343(3)	97(2)
C(5)	12127(4)	3953(3)	-577(3)	103(2)
C(6)	11179(3)	3377(3)	-584(2)	78(1)
C(7)	10598(3)	3549(2)	188(2)	68(1)
C(8)	9671(2)	1819(2)	2324(2)	43(1)
C(9)	8901(4)	1369(2)	1561(2)	78(1)
C(10)	8259(4)	717(2)	1910(3)	90(1)
C(11)	9073(4)	161(2)	2542(4)	94(2)
C(12)	9832(3)	614(2)	3306(3)	85(1)
C(13)	10478(3)	1263(2)	2947(3)	73(1)
C(14)	10039(2)	3402(2)	3112(2)	40(1)
C(15)	10899(2)	3567(2)	3911(2)	42(1)
C(16)	10584(2)	3730(2)	4719(2)	44(1)
C(17)	9467(2)	3767(2)	4782(2)	42(1)
C(18)	8631(3)	3659(2)	3976(2)	44(1)
C(19)	8901(2)	3476(2)	3148(2)	42(1)
C(20)	12123(2)	3585(2)	3895(2)	44(1)
C(21)	12711(3)	2958(2)	3638(2)	63(1)
C(22)	13834(3)	3024(2)	3618(3)	76(1)
C(23)	14413(3)	3711(3)	3855(3)	75(1)
C(24)	13849(3)	4341(2)	4112(3)	70(1)
C(25)	12727(3)	4288(2)	4146(2)	55(1)

C(26)	9157(2)	3888(2)	5674(2)	43(1)
C(27)	9856(3)	4335(2)	6370(2)	51(1)
C(28)	9579(3)	4410(2)	7216(2)	61(1)
C(29)	8628(4)	4059(2)	7372(2)	68(1)
C(30)	7932(3)	3621(2)	6696(2)	68(1)
C(31)	8201(3)	3538(2)	5857(2)	56(1)
C(32)	7941(2)	3370(2)	2317(2)	43(1)
C(33)	7972(3)	3707(2)	1478(2)	58(1)
C(34)	7072(3)	3606(2)	726(2)	73(1)
C(35)	6141(4)	3181(3)	803(3)	79(1)
C(36)	6089(3)	2848(2)	1620(3)	71(1)
C(37)	6988(3)	2943(2)	2370(2)	57(1)

Table 3A. Bond lengths [Å].

N(1)-C(1)	1.379(4)
N(1)-C(2)	1.450(4)
N(1)-H(1)	0.8600
N(2)-C(1)	1.283(3)
N(2)-C(8)	1.462(4)
C(1)-C(14)	1.498(4)
C(2)-C(3)	1.502(4)
C(2)-C(7)	1.509(4)
C(2)-H(2)	0.9800
C(3)-C(4)	1.519(5)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.514(6)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.500(5)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.516(5)
C(6)-H(6A)	0.9700

C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-C(9)	1.502(4)
C(8)-C(13)	1.510(4)
C(8)-H(8)	0.9800
C(9)-C(10)	1.509(5)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(10)-C(11)	1.520(6)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.498(6)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.515(5)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(19)	1.395(4)
C(14)-C(15)	1.418(4)
C(15)-C(16)	1.382(4)
C(15)-C(20)	1.485(4)
C(16)-C(17)	1.377(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.394(4)
C(17)-C(26)	1.485(4)
C(18)-C(19)	1.390(4)
C(18)-H(18)	0.9300
C(19)-C(32)	1.503(4)
C(20)-C(21)	1.379(4)
C(20)-C(25)	1.398(4)
C(21)-C(22)	1.370(5)

Table 3A. Bond lengths [Å] continued.

C(21)-H(21)	0.9300
C(22)-C(23)	1.357(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.367(5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.372(4)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-C(31)	1.382(4)
C(26)-C(27)	1.400(4)
C(27)-C(28)	1.390(4)
C(27)-H(27)	0.9300
C(28)-C(29)	1.361(5)
C(28)-H(28)	0.9300
C(29)-C(30)	1.373(5)
C(29)-H(29)	0.9300
C(30)-C(31)	1.378(4)
C(30)-H(30)	0.9300
C(31)-H(31)	0.9300
C(32)-C(37)	1.376(4)
C(32)-C(33)	1.389(4)
C(33)-C(34)	1.383(4)
C(33)-H(33)	0.9300
C(34)-C(35)	1.361(5)
C(34)-H(34)	0.9300
C(35)-C(36)	1.363(5)
C(35)-H(35)	0.9300
C(36)-C(37)	1.379(5)
C(36)-H(36)	0.9300
C(37)-H(37)	0.9300

Table 3B. Bond angles [°].

C(1)-N(1)-C(2)	122.9(2)
C(1)-N(1)-H(1)	118.6
C(2)-N(1)-H(1)	118.6
C(1)-N(2)-C(8)	120.5(2)
N(2)-C(1)-N(1)	119.8(3)
N(2)-C(1)-C(14)	126.2(3)
N(1)-C(1)-C(14)	114.0(2)
N(1)-C(2)-C(3)	111.0(3)
N(1)-C(2)-C(7)	112.1(3)
C(3)-C(2)-C(7)	110.9(3)
N(1)-C(2)-H(2)	107.5
C(3)-C(2)-H(2)	107.5
C(7)-C(2)-H(2)	107.5
C(2)-C(3)-C(4)	110.7(3)
C(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(5)-C(4)-C(3)	110.7(4)
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(6)-C(5)-C(4)	110.3(3)
C(6)-C(5)-H(5A)	109.6
C(4)-C(5)-H(5A)	109.6
C(6)-C(5)-H(5B)	109.6
C(4)-C(5)-H(5B)	109.6
H(5A)-C(5)-H(5B)	108.1
C(5)-C(6)-C(7)	111.1(3)
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6A)	109.4

C(5)-C(6)-H(6B)	109.4
C(7)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(2)-C(7)-C(6)	111.3(3)
C(2)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7A)	109.4
C(2)-C(7)-H(7B)	109.4
C(6)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
N(2)-C(8)-C(9)	108.8(2)
N(2)-C(8)-C(13)	112.5(3)
C(9)-C(8)-C(13)	110.7(3)
N(2)-C(8)-H(8)	108.3
C(9)-C(8)-H(8)	108.3
C(13)-C(8)-H(8)	108.3
C(8)-C(9)-C(10)	112.4(3)
C(8)-C(9)-H(9A)	109.1
C(10)-C(9)-H(9A)	109.1
C(8)-C(9)-H(9B)	109.1
C(10)-C(9)-H(9B)	109.1

Table 3B. Bond angles [°] continued.

H(9A)-C(9)-H(9B)	107.8
C(9)-C(10)-C(11)	110.8(3)
C(9)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
C(12)-C(11)-C(10)	110.8(3)
C(12)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(11)-C(12)-C(13)	111.8(4)

C(11)-C(12)-H(12A)	109.3
C(13)-C(12)-H(12A)	109.3
C(11)-C(12)-H(12B)	109.3
C(13)-C(12)-H(12B)	109.3
H(12A)-C(12)-H(12B)	107.9
C(8)-C(13)-C(12)	110.9(3)
C(8)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13A)	109.5
C(8)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	108.0
C(19)-C(14)-C(15)	119.0(3)
C(19)-C(14)-C(1)	122.4(3)
C(15)-C(14)-C(1)	118.6(3)
C(16)-C(15)-C(14)	118.8(3)
C(16)-C(15)-C(20)	119.3(3)
C(14)-C(15)-C(20)	121.9(3)
C(17)-C(16)-C(15)	123.1(3)
C(17)-C(16)-H(16)	118.5
C(15)-C(16)-H(16)	118.5
C(16)-C(17)-C(18)	117.3(3)
C(16)-C(17)-C(26)	121.7(3)
C(18)-C(17)-C(26)	121.0(3)
C(19)-C(18)-C(17)	122.0(3)
C(19)-C(18)-H(18)	119.0
C(17)-C(18)-H(18)	119.0
C(18)-C(19)-C(14)	119.6(3)
C(18)-C(19)-C(32)	118.1(3)
C(14)-C(19)-C(32)	122.3(3)
C(21)-C(20)-C(25)	117.1(3)
C(21)-C(20)-C(15)	124.6(3)
C(25)-C(20)-C(15)	118.3(3)
C(22)-C(21)-C(20)	121.4(4)
C(22)-C(21)-H(21)	119.3
C(20)-C(21)-H(21)	119.3
C(23)-C(22)-C(21)	121.2(4)
C(23)-C(22)-H(22)	119.4
C(21)-C(22)-H(22)	119.4

C(22)-C(23)-C(24)	118.5(4)
C(22)-C(23)-H(23)	120.7

Table 3B. Bond angles [°] continued.

C(24)-C(23)-H(23)	120.7
C(23)-C(24)-C(25)	121.5(4)
C(23)-C(24)-H(24)	119.3
C(25)-C(24)-H(24)	119.3
C(24)-C(25)-C(20)	120.3(3)
C(24)-C(25)-H(25)	119.8
C(20)-C(25)-H(25)	119.8
C(31)-C(26)-C(27)	117.9(3)
C(31)-C(26)-C(17)	121.3(3)
C(27)-C(26)-C(17)	120.7(3)
C(28)-C(27)-C(26)	119.9(3)
C(28)-C(27)-H(27)	120.1
C(26)-C(27)-H(27)	120.1
C(29)-C(28)-C(27)	120.6(3)
C(29)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(28)-C(29)-C(30)	120.3(3)
C(28)-C(29)-H(29)	119.9
C(30)-C(29)-H(29)	119.9
C(29)-C(30)-C(31)	119.6(3)
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-H(30)	120.2
C(30)-C(31)-C(26)	121.7(3)
C(30)-C(31)-H(31)	119.1
C(26)-C(31)-H(31)	119.1
C(37)-C(32)-C(33)	117.8(3)
C(37)-C(32)-C(19)	120.6(3)
C(33)-C(32)-C(19)	121.6(3)
C(34)-C(33)-C(32)	120.4(3)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(35)-C(34)-C(33)	120.3(4)

C(35)-C(34)-H(34)	119.9
C(33)-C(34)-H(34)	119.9
C(34)-C(35)-C(36)	120.4(3)
C(34)-C(35)-H(35)	119.8
C(36)-C(35)-H(35)	119.8
C(35)-C(36)-C(37)	119.6(4)
C(35)-C(36)-H(36)	120.2
C(37)-C(36)-H(36)	120.2
C(32)-C(37)-C(36)	121.6(3)
C(32)-C(37)-H(37)	119.2
C(36)-C(37)-H(37)	119.2

Table 3C. Selected torsion angles [°].

-176.53	(0.25)	C8 - N2 - C1 - N1
4.51	(0.45)	C8 - N2 - C1 - C14
-7.86	(0.43)	C2 - N1 - C1 - N2
171.21	(0.25)	C2 - N1 - C1 - C14
-150.50	(0.30)	C1 - N1 - C2 - C3
84.80	(0.36)	C1 - N1 - C2 - C7
178.55	(0.34)	N1 - C2 - C3 - C4
-56.07	(0.45)	C7 - C2 - C3 - C4
57.36	(0.51)	C2 - C3 - C4 - C5
-57.50	(0.54)	C3 - C4 - C5 - C6
56.67	(0.52)	C4 - C5 - C6 - C7
-179.94	(0.28)	N1 - C2 - C7 - C6
55.32	(0.40)	C3 - C2 - C7 - C6
-55.83	(0.46)	C5 - C6 - C7 - C2
137.31	(0.31)	C1 - N2 - C8 - C9
-99.74	(0.35)	C1 - N2 - C8 - C13
179.37	(0.32)	N2 - C8 - C9 - C10
55.33	(0.44)	C13 - C8 - C9 - C10
-55.08	(0.49)	C8 - C9 - C10 - C11
54.74	(0.47)	C9 - C10 - C11 - C12
-55.93	(0.48)	C10 - C11 - C12 - C13
-176.98	(0.31)	N2 - C8 - C13 - C12
-55.10	(0.43)	C9 - C8 - C13 - C12
56.35	(0.48)	C11 - C12 - C13 - C8

-69.37	(0.41)	N2 - C1 - C14 - C19
111.63	(0.31)	N1 - C1 - C14 - C19
108.71	(0.34)	N2 - C1 - C14 - C15
-70.29	(0.34)	N1 - C1 - C14 - C15
5.34	(0.41)	C19 - C14 - C15 - C16
-172.80	(0.25)	C1 - C14 - C15 - C16
-173.24	(0.26)	C19 - C14 - C15 - C20
8.62	(0.40)	C1 - C14 - C15 - C20
-2.16	(0.44)	C14 - C15 - C16 - C17
176.46	(0.27)	C20 - C15 - C16 - C17
-2.24	(0.44)	C15 - C16 - C17 - C18
175.60	(0.26)	C15 - C16 - C17 - C26
3.54	(0.42)	C16 - C17 - C18 - C19
-174.31	(0.26)	C26 - C17 - C18 - C19
-0.37	(0.42)	C17 - C18 - C19 - C14
179.91	(0.25)	C17 - C18 - C19 - C32
-4.11	(0.41)	C15 - C14 - C19 - C18
173.95	(0.26)	C1 - C14 - C19 - C18
175.59	(0.25)	C15 - C14 - C19 - C32
-6.35	(0.42)	C1 - C14 - C19 - C32
122.63	(0.34)	C16 - C15 - C20 - C21
-58.80	(0.42)	C14 - C15 - C20 - C21
-58.29	(0.38)	C16 - C15 - C20 - C25
120.29	(0.31)	C14 - C15 - C20 - C25
-0.79	(0.50)	C25 - C20 - C21 - C22
178.31	(0.32)	C15 - C20 - C21 - C22
0.25	(0.60)	C20 - C21 - C22 - C23
-0.30	(0.60)	C21 - C22 - C23 - C24
0.94	(0.57)	C22 - C23 - C24 - C25
-1.52	(0.52)	C23 - C24 - C25 - C20

Table 3C. Selected torsion angles [°] continued.

1.40	(0.46)	C21 - C20 - C25 - C24
-177.75	(0.29)	C15 - C20 - C25 - C24
-145.75	(0.30)	C16 - C17 - C26 - C31
32.01	(0.42)	C18 - C17 - C26 - C31
31.50	(0.43)	C16 - C17 - C26 - C27

-150.74	(0.29)	C18 - C17 - C26 - C27
0.39	(0.44)	C31 - C26 - C27 - C28
-176.95	(0.28)	C17 - C26 - C27 - C28
-0.62	(0.48)	C26 - C27 - C28 - C29
0.46	(0.54)	C27 - C28 - C29 - C30
-0.07	(0.56)	C28 - C29 - C30 - C31
-0.15	(0.54)	C29 - C30 - C31 - C26
-0.02	(0.47)	C27 - C26 - C31 - C30
177.31	(0.31)	C17 - C26 - C31 - C30
-43.53	(0.39)	C18 - C19 - C32 - C37
136.77	(0.31)	C14 - C19 - C32 - C37
135.20	(0.30)	C18 - C19 - C32 - C33
-44.50	(0.41)	C14 - C19 - C32 - C33
-0.58	(0.47)	C37 - C32 - C33 - C34
-179.34	(0.29)	C19 - C32 - C33 - C34
0.66	(0.54)	C32 - C33 - C34 - C35
-0.34	(0.60)	C33 - C34 - C35 - C36
-0.04	(0.60)	C34 - C35 - C36 - C37
0.20	(0.47)	C33 - C32 - C37 - C36
178.97	(0.30)	C19 - C32 - C37 - C36
0.11	(0.55)	C35 - C36 - C37 - C32

Table 4. Selected contact distances [Å] and angles [°] and best plane calculations.

Specified potential hydrogen bonds (with esds except fixed and riding H)

D-H	H...A	D...A	<(DHA)	
0.86	2.72	3.563(4)	166.1	N1-H1...C28_$1
0.86	2.27	3.054(4)	151.1	N1-H1...H28_$1

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

8.8439 (0.0132) x - 4.2088 (0.0249) y + 6.6908 (0.0274) z = 9.3506 (0.0090)

*	0.0124 (0.0009)	C2
*	-0.0345 (0.0018)	N1
*	0.0355 (0.0019)	C1
*	-0.0052 (0.0021)	N2
*	-0.0082 (0.0015)	C8

Rms deviation of fitted atoms = 0.0232

0.6002 (0.0141) x + 16.4461 (0.0073) y - 3.3465 (0.0163) z = 5.1876 (0.0141)

Angle to previous plane (with approximate esd) = 69.82 (0.11)

*	-0.0308 (0.0020)	C14
*	0.0237 (0.0020)	C15
*	0.0035 (0.0020)	C16
*	-0.0240 (0.0020)	C17
*	0.0172 (0.0020)	C18
*	0.0105 (0.0019)	C19

Rms deviation of fitted atoms = 0.0204

0.5509 (0.0168) x - 5.1919 (0.0233) y + 13.6998 (0.0103) z = 4.1476 (0.0221)

Angle to previous plane (with approximate esd) = 59.70 (0.11)

*	-0.0048 (0.0022)	C20
*	0.0007 (0.0025)	C21