SUPPORTING INFORMATION

Synthesis and Characterization of μ-η^1-η^1-3,5-Di-*tert*-butylpyrazolate Derivatives of Aluminum

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Figure 1: Ortep plot of [η^1-η^1-3,5-tBu$_2$pz(μ-Al)Me$_2$]$_2$ (**1**).

Table 1: Crystal data and structure refinement for **1**.

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

Table 3: Bond lengths and angles for **1**.

Table 4: Anisotropic displacement parameters (Å^2 x 10^3) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Table 5: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **1**.

Figure 2: Ortep plot of [η^1-η^1-3,5-tBu$_2$pz(μ-Al)Cl$_2$]$_2$ (**3**).

Table 6: Crystal data and structure refinement for **3**.

Table 7: 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 Uij tensor.

Table 8: Bond lengths and angles for **3**.

Table 9: 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 U11 + ... + 2 h k a* b* U12].

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

Figure 3: Ortep plot of [(η^1-η^1-3,5-*t*Bupz)$_2$(μ-S)(μ-Al)(C≡CPh)$_2$] (**6**).

Table 11: Crystal data and structure refinement for **6**.

Table 12: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 13: Bond lengths and angles for **6**.

Table 14: Anisotropic displacement parameters ($Å^2$ x 10^3) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Table 15: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **6**.

Figure 4: Ortep plot of [(η^1-η^1-3,5-*t*Bupz)$_2$(μ-Se)(μ-Al)(C≡CPh)$_2$] (**7**).

Table 16: Crystal data and structure refinement for **7**.

Table 17: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **7**. U(eq)

is defined as one third of the trace of the orthogonalized Uij tensor.

Table 18: Bond lengths and angles for **7**.

Table 19: Anisotropic displacement parameters ($Å^2$ x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Table 20: Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **7**.

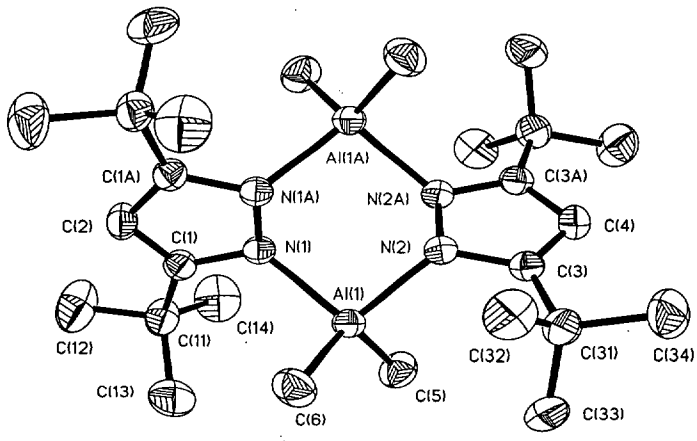

Figure 1: Ortep plot of $[\eta^1\text{-}\eta^1\text{-}3,5\text{-}t\mathrm{Bu}_2\mathrm{pz}(\mu\text{-}\mathrm{Al})\mathrm{Me}_2]_2$ (**1**).

Table 1. Crystal Data and Structure Refinement for **1**.

Empirical formula	C26 H50 Al2 N4
Formula weight	472.66
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	*Pbcn*
Unit cell dimensions	a = 9.3230(10) Å alpha = 90 deg. b = 20.403(3) Å beta = 90 deg. c = 16.186(3) Å gamma = 90 deg.
Volume, Z	3078.9(8) Å^3, 4
Density (calculated)	1.020 Mg/m^3
Absorption coefficient	0.113 mm^-1
F(000)	1040
Crystal size	0.60 x 0.60 x 0.50 mm
Theta range for data collection	3.71 to 25.04 deg.
Limiting indices	-10<=h<=11, -24<=k<=24, -19<=l<=19
Reflections collected	5656
Independent reflections	2718 [*R*(int) = 0.0184]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2714 / 0 / 154
Goodness-of-fit on F^2	1.053
Final R indices [I>2sigma(I)]	*R*1 = 0.0384, *wR*2 = 0.1027
R indices (all data)	*R*1 = 0.0469, *wR*2 = 0.1130
Largest diff. peak and hole	0.211 and -0.192 e.Å^-3

Table 2. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for **1**.

	x	y	z	U(eq)
Al(1)	1879(1)	3692(1)	7395(1)	28(1)
N(1)	485(1)	2992(1)	7170(1)	28(1)
N(2)	572(1)	4383(1)	7781(1)	30(1)
C(1)	751(2)	2361(1)	6966(1)	32(1)
C(2)	0	1957(1)	7500	36(1)
C(3)	889(2)	5014(1)	7960(1)	32(1)
C(4)	0	5417(1)	7500	36(1)
C(5)	2724(2)	4092(1)	6405(1)	43(1)
C(6)	3070(2)	3300(1)	8263(1)	46(1)
C(11)	1686(2)	2166(1)	6234(1)	42(1)
C(12)	1462(3)	1441(1)	6045(2)	75(1)
C(13)	3279(2)	2271(1)	6428(1)	59(1)
C(14)	1249(3)	2570(1)	5482(1)	62(1)
C(31)	2021(2)	5207(1)	8589(1)	38(1)
C(32)	1871(2)	4781(1)	9362(1)	53(1)
C(34)	1809(2)	5926(1)	8834(1)	60(1)
C(33)	3530(2)	5127(1)	8224(1)	47(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 3. Bond Lengths [Å] and Angles [°] for **1**.

Al(1)-C(6)	1.962(2)
Al(1)-C(5)	1.963(2)
Al(1)-N(2)	1.9651(13)
Al(1)-N(1)	1.9638(13)
N(1)-C(1)	1.353(2)
N(1)-N(1)#1	1.399(2)
N(2)-C(3)	1.352(2)
N(2)-N(2)#1	1.401(2)
C(1)-C(2)	1.385(2)
C(1)-C(11)	1.523(2)
C(2)-C(1)#1	1.385(2)
C(3)-C(4)	1.386(2)
C(3)-C(31)	1.519(2)
C(4)-C(3)#1	1.386(2)
C(11)-C(12)	1.526(2)
C(11)-C(14)	1.526(3)
C(11)-C(13)	1.533(3)
C(31)-C(32)	1.529(3)
C(31)-C(34)	1.533(2)
C(31)-C(33)	1.534(2)
C(6)-Al(1)-C(5)	121.80(9)
C(6)-Al(1)-N(1)	102.17(7)
C(5)-Al(1)-N(1)	114.67(7)
C(6)-Al(1)-N(2)	114.56(7)
C(5)-Al(1)-N(2)	102.09(7)
N(1)-Al(1)-N(2)	99.77(6)
C(1)-N(1)-N(1)#1	107.78(8)
C(1)-N(1)-Al(1)	127.98(11)
N(1)#1-N(1)-Al(1)	106.66(8)
C(3)-N(2)-N(2)#1	107.79(8)
C(3)-N(2)-Al(1)	128.00(10)
N(2)#1-N(2)-Al(1)	105.42(8)
N(1)-C(1)-C(2)	108.73(14)
N(1)-C(1)-C(11)	122.97(13)
C(2)-C(1)-C(11)	128.25(14)
C(1)#1-C(2)-C(1)	106.9(2)
N(2)-C(3)-C(4)	108.66(14)
N(2)-C(3)-C(31)	122.91(14)
C(4)-C(3)-C(31)	128.4(2)
C(3)-C(4)-C(3)#1	107.0(2)
C(1)-C(11)-C(12)	109.35(14)
C(1)-C(11)-C(14)	109.1(2)
C(12)-C(11)-C(14)	109.0(2)
C(1)-C(11)-C(13)	111.0(2)
C(12)-C(11)-C(13)	108.0(2)
C(14)-C(11)-C(13)	110.3(2)
C(3)-C(31)-C(32)	109.66(14)
C(3)-C(31)-C(34)	109.43(14)
C(32)-C(31)-C(34)	108.7(2)
C(3)-C(31)-C(33)	110.54(14)
C(32)-C(31)-C(33)	109.8(2)
C(34)-C(31)-C(33)	108.7(2)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+3/2

Table 4. Anisotropic Displacement Parameters ($Å^2$ x 10^3) for **1**.

	U11	U22	U33	U23	U13	U12
Al(1)	25(1)	29(1)	31(1)	2(1)	1(1)	0(1)
N(1)	27(1)	28(1)	29(1)	0(1)	6(1)	0(1)
N(2)	26(1)	29(1)	36(1)	-1(1)	-2(1)	0(1)
C(1)	33(1)	29(1)	33(1)	-3(1)	5(1)	0(1)
C(2)	45(1)	24(1)	39(1)	0	10(1)	0
C(3)	28(1)	31(1)	37(1)	-3(1)	3(1)	-1(1)
C(4)	37(1)	26(1)	46(1)	0	3(1)	0
C(5)	44(1)	41(1)	43(1)	3(1)	8(1)	-7(1)
C(6)	44(1)	45(1)	48(1)	3(1)	-11(1)	8(1)
C(11)	52(1)	33(1)	40(1)	-4(1)	18(1)	-1(1)
C(12)	104(2)	44(1)	76(2)	-22(1)	50(2)	-10(1)
C(13)	50(1)	62(1)	64(1)	-3(1)	26(1)	10(1)
C(14)	85(2)	68(1)	33(1)	-5(1)	10(1)	3(1)
C(31)	37(1)	36(1)	42(1)	-8(1)	-4(1)	-3(1)
C(32)	61(1)	62(1)	37(1)	-5(1)	-3(1)	-5(1)
C(34)	63(1)	45(1)	71(1)	-23(1)	-15(1)	2(1)
C(33)	35(1)	48(1)	58(1)	-7(1)	-4(1)	-9(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Table 5. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for **1**.

	x	y	z	U(eq)
H(2A)	0	1496(1)	7500	43
H(4A)	0	5878(1)	7500	43
H(5A)	3424(10)	3795(3)	6167(5)	64
H(5B)	3191(12)	4500(3)	6555(2)	64
H(5C)	1975(3)	4180(6)	6004(3)	64
H(6A)	3524(11)	2906(4)	8052(3)	69
H(6B)	2474(3)	3189(6)	8734(3)	69
H(6C)	3802(9)	3610(3)	8431(6)	69
H(12A)	2006(17)	1322(2)	5556(7)	112
H(12B)	451(4)	1359(2)	5948(11)	112
H(12C)	1786(19)	1180(1)	6510(5)	112
H(13A)	3855(2)	2109(7)	5973(4)	88
H(13B)	3528(4)	2035(6)	6929(5)	88
H(13C)	3463(4)	2735(1)	6506(9)	88
H(14A)	1857(11)	2456(6)	5017(3)	93
H(14B)	1354(16)	3032(1)	5605(4)	93
H(14C)	256(6)	2477(6)	5344(6)	93
H(32A)	2601(10)	4902(5)	9760(4)	80
H(32B)	1987(15)	4324(1)	9212(2)	80
H(32C)	929(6)	4846(5)	9603(5)	80
H(34A)	2487(12)	6041(2)	9265(7)	89
H(34B)	839(6)	5989(2)	9036(9)	89
H(34C)	1967(17)	6204(1)	8357(3)	89
H(33A)	4237(2)	5265(6)	8628(3)	70
H(33B)	3617(5)	5395(5)	7732(4)	70
H(33C)	3688(5)	4671(1)	8083(7)	70

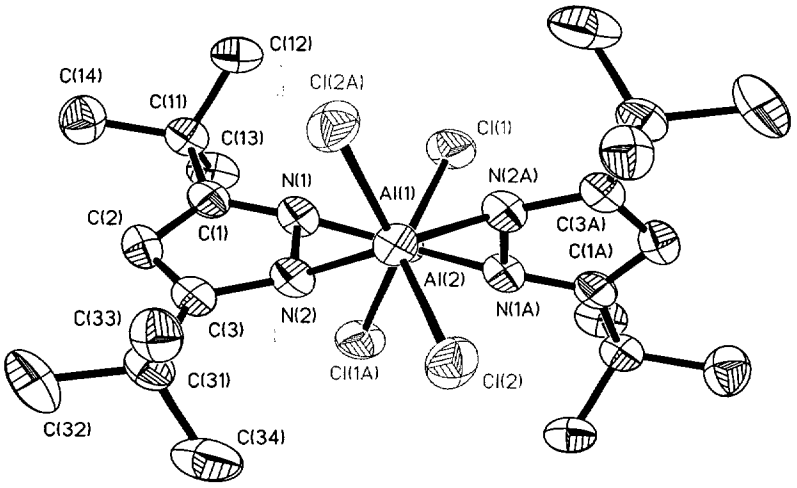

Figure 2. Ortep plot of $[\eta^1\text{-}\eta^1\text{-}3,5\text{-}t\mathrm{Bu}_2\mathrm{pz}(\mu\text{-}\mathrm{Al})\mathrm{Cl}_2]_2$ (**3**).

Table 6. Crystal Data and Structure Refinement for **3**.

Empirical formula	C22 H38 Al2 Cl4 N4
Formula weight	554.32
Temperature	203(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbcn
Unit cell dimensions	a = 13.171(3) Å alpha = 90 deg. b = 17.706(4) Å beta = 90 deg. c = 12.870(2) Å gamma = 90 deg.
Volume, Z	3001.3(11) Å^3, 4
Density (calculated)	1.227 Mg/m^3
Absorption coefficient	0.470 mm^-1
F(000)	1168
Crystal size	0.90 x 0.60 x 0.30 mm
Theta range for data collection	3.52 to 25.05 deg.
Limiting indices	-15<=h<=15, -21<=k<=10, -15<=l<=15
Reflections collected	4438
Independent reflections	2655 [R(int) = 0.0564]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2651 / 0 / 152
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	*R*1 = 0.0427, *wR*2 = 0.1061
R indices (all data)	*R*1 = 0.0559, *wR*2 = 0.1242
Largest diff. peak and hole	0.319 and -0.343 e.Å^-3

Table 7. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
Al(1)	5000	2407(1)	2500	32(1)
Al(2)	5000	494(1)	2500	33(1)
Cl(1)	3715(1)	3074(1)	2130(1)	52(1)
Cl(2)	5612(1)	-138(1)	3737(1)	54(1)
N(1)	5431(1)	1751(1)	1413(2)	34(1)
N(2)	5975(1)	1150(1)	1878(2)	35(1)
C(1)	5882(2)	1912(1)	495(2)	36(1)
C(2)	6717(2)	1441(1)	373(2)	38(1)
C(3)	6759(2)	974(1)	1234(2)	35(1)
C(11)	5484(2)	2482(1)	-286(2)	39(1)
C(12)	4342(2)	2340(2)	-464(2)	47(1)
C(13)	5684(2)	3296(1)	82(3)	48(1)
C(14)	6035(2)	2372(2)	-1323(2)	56(1)
C(31)	7548(2)	367(1)	1461(2)	42(1)
C(32)	8391(2)	419(2)	638(3)	63(1)
C(33)	7088(2)	-429(1)	1385(2)	45(1)
C(34)	8000(2)	500(2)	2546(3)	67(1)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 8. Bond Lengths [Å] and Angles [°] for **3**.

Al(1)-N(1)#1	1.904(2)
Al(1)-N(1)	1.904(2)
Al(1)-Cl(1)#1	2.1181(9)
Al(1)-Cl(1)	2.1181(9)
Al(2)-N(2)#1	1.907(2)
Al(2)-N(2)	1.907(2)
Al(2)-Cl(2)#1	2.1062(9)
Al(2)-Cl(2)	2.1062(9)
N(1)-C(1)	1.353(3)
N(1)-N(2)	1.416(3)
N(2)-C(3)	1.360(3)
C(1)-C(2)	1.389(3)
C(1)-C(11)	1.518(3)
C(2)-C(3)	1.384(4)
C(3)-C(31)	1.524(3)
C(11)-C(14)	1.532(4)
C(11)-C(13)	1.540(3)
C(11)-C(12)	1.541(4)
C(31)-C(32)	1.537(4)
C(31)-C(34)	1.536(4)
C(31)-C(33)	1.537(4)
N(1)#1-Al(1)-N(1)	104.86(12)
N(1)#1-Al(1)-Cl(1)#1	114.36(6)
N(1)-Al(1)-Cl(1)#1	105.51(6)
N(1)#1-Al(1)-Cl(1)	105.51(6)
N(1)-Al(1)-Cl(1)	114.36(6)
Cl(1)#1-Al(1)-Cl(1)	112.22(6)
N(2)#1-Al(2)-N(2)	105.02(12)
N(2)#1-Al(2)-Cl(2)#1	112.52(6)
N(2)-Al(2)-Cl(2)#1	105.31(7)
N(2)#1-Al(2)-Cl(2)	105.31(7)
N(2)-Al(2)-Cl(2)	112.52(6)
Cl(2)#1-Al(2)-Cl(2)	115.78(6)
C(1)-N(1)-N(2)	107.7(2)
C(1)-N(1)-Al(1)	130.1(2)
N(2)-N(1)-Al(1)	107.4(2)
C(3)-N(2)-N(1)	107.4(2)
C(3)-N(2)-Al(2)	128.9(2)
N(1)-N(2)-Al(2)	107.06(13)
N(1)-C(1)-C(2)	108.7(2)
N(1)-C(1)-C(11)	124.5(2)
C(2)-C(1)-C(11)	126.7(2)
C(3)-C(2)-C(1)	107.4(2)
N(2)-C(3)-C(2)	108.7(2)
N(2)-C(3)-C(31)	124.2(2)
C(2)-C(3)-C(31)	127.0(2)
C(1)-C(11)-C(14)	109.2(2)
C(1)-C(11)-C(13)	111.1(2)
C(14)-C(11)-C(13)	107.8(2)
C(1)-C(11)-C(12)	109.1(2)
C(14)-C(11)-C(12)	108.2(2)
C(13)-C(11)-C(12)	111.4(2)
C(3)-C(31)-C(32)	108.5(2)
C(3)-C(31)-C(34)	109.3(2)
C(32)-C(31)-C(34)	109.7(2)
C(3)-C(31)-C(33)	111.5(2)
C(32)-C(31)-C(33)	107.2(2)
C(34)-C(31)-C(33)	110.5(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Table 9. Anisotropic Displacement Parameters ($Å^2$ x 10^3) for **3**.

	U11	U22	U33	U23	U13	U12
Al(1)	28(1)	25(1)	44(1)	0	-1(1)	0
Al(2)	39(1)	25(1)	34(1)	0	1(1)	0
Cl(1)	45(1)	53(1)	58(1)	-6(1)	-7(1)	21(1)
Cl(2)	60(1)	58(1)	43(1)	15(1)	4(1)	17(1)
N(1)	33(1)	25(1)	45(1)	4(1)	3(1)	3(1)
N(2)	34(1)	25(1)	45(1)	0(1)	2(1)	4(1)
C(1)	32(1)	30(1)	45(2)	-1(1)	1(1)	-4(1)
C(2)	34(1)	34(1)	46(2)	-4(1)	8(1)	-1(1)
C(3)	31(1)	29(1)	45(1)	-4(1)	1(1)	-1(1)
C(11)	37(1)	34(1)	45(2)	5(1)	-1(1)	0(1)
C(12)	44(2)	45(2)	52(2)	0(1)	-11(1)	-6(1)
C(13)	46(2)	34(1)	64(2)	7(1)	-11(1)	-4(1)
C(14)	63(2)	55(2)	50(2)	14(1)	9(2)	5(1)
C(31)	35(1)	35(1)	55(2)	-3(1)	0(1)	7(1)
C(32)	42(2)	46(2)	99(3)	4(2)	20(2)	10(1)
C(33)	49(2)	34(1)	52(2)	2(1)	6(1)	10(1)
C(34)	52(2)	62(2)	86(2)	-16(2)	-26(2)	16(2)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Table 10. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for **3**.

	x	y	z	U(eq)
H(2A)	7171(2)	1440(1)	-191(2)	46
H(12A)	3975(3)	2432(11)	177(5)	70
H(12B)	4239(2)	1821(4)	-680(15)	70
H(12C)	4095(4)	2678(8)	-1000(11)	70
H(13A)	6401(3)	3358(4)	228(16)	72
H(13B)	5294(12)	3395(4)	706(9)	72
H(13C)	5482(15)	3647(2)	-459(7)	72
H(14A)	6754(3)	2468(11)	-1231(4)	84
H(14B)	5763(11)	2720(9)	-1833(5)	84
H(14C)	5937(13)	1857(4)	-1563(8)	84
H(32A)	8108(4)	314(13)	-43(4)	94
H(32B)	8918(9)	53(10)	794(11)	94
H(32C)	8679(13)	923(5)	643(13)	94
H(33A)	6790(13)	-498(4)	703(5)	68
H(33B)	6568(10)	-488(4)	1912(10)	68
H(33C)	7617(3)	-803(1)	1492(15)	68
H(34C)	8338(16)	986(7)	2562(6)	100
H(34D)	8486(14)	104(8)	2702(9)	100
H(34A)	7460(3)	493(14)	3059(4)	100

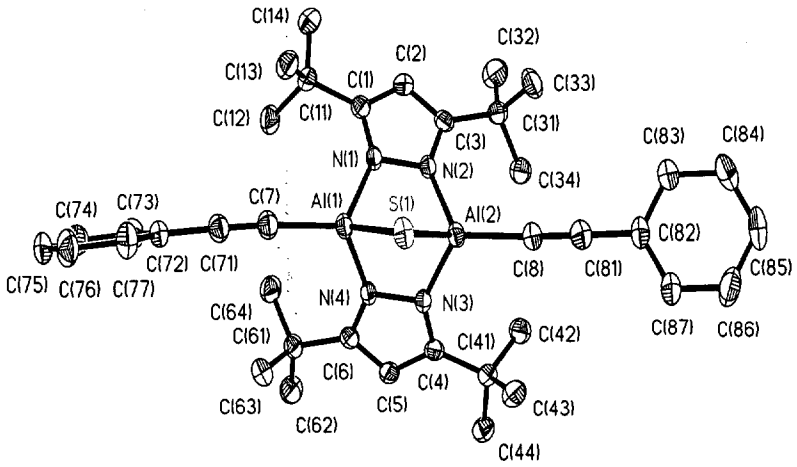

Figure 3. Ortep plot of [(η^1-η^1-3,5-tBupz)$_2$(μ-S)(μ-Al)(C≡CPh)$_2$] (**6**).

Table 11. Crystal Data and Structure Refinement for **3**.

Empirical formula	C52 H64 Al2 N4 S
Formula weight	831.09
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 18.260(3) A alpha = 90 deg. b = 15.835(7) A beta = 115.590(12) deg. c = 18.652(4) A gamma = 90 deg.
Volume, Z	4864(2) A^3, 4
Density (calculated)	1.135 Mg/m^3
Absorption coefficient	0.140 mm^-1
F(000)	1784
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	3.53 to 25.03 deg.
Limiting indices	-21<=h<=21, -12<=k<=18, -19<=l<=22
Reflections collected	9561
Independent reflections	8530 [R(int) = 0.0528]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8491 / 0 / 546
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0563, wR2 = 0.1148
R indices (all data)	R1 = 0.0791, wR2 = 0.1415
Largest diff. peak and hole	0.800 and -0.816 e.A^-3

Table 12. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for **3**.

	x	y	z	U(eq)
S(1)	2605(1)	7344(1)	3652(1)	31(1)
Al(1)	3398(1)	7084(1)	3066(1)	25(1)
N(1)	2637(1)	7252(1)	1965(1)	25(1)
C(1)	2373(2)	6895(2)	1237(2)	28(1)
Al(2)	2394(1)	8481(1)	2915(1)	24(1)
N(2)	2206(1)	8013(1)	1879(1)	24(1)
C(2)	1798(2)	7418(2)	688(2)	31(1)
N(3)	3507(1)	8845(1)	3240(1)	25(1)
C(3)	1704(2)	8109(2)	1094(2)	27(1)
N(4)	3993(1)	8154(1)	3242(1)	25(1)
C(4)	3990(2)	9537(2)	3482(2)	26(1)
C(5)	4771(2)	9299(2)	3625(2)	29(1)
C(6)	4756(2)	8446(2)	3465(2)	26(1)
C(7)	4053(2)	6087(2)	3334(2)	32(1)
C(8)	1615(2)	9275(2)	2923(2)	31(1)
C(11)	2640(2)	6039(2)	1072(2)	32(1)
C(12)	3543(2)	6048(2)	1252(2)	42(1)
C(13)	2474(2)	5363(2)	1574(2)	41(1)
C(14)	2152(2)	5818(2)	193(2)	48(1)
C(31)	1120(2)	8838(2)	732(2)	33(1)
C(32)	880(2)	8865(2)	-166(2)	51(1)
C(33)	356(2)	8691(2)	863(2)	48(1)
C(34)	1509(2)	9683(2)	1086(2)	37(1)
C(41)	3710(2)	10407(2)	3596(2)	30(1)
C(42)	3064(2)	10756(2)	2806(2)	39(1)
C(43)	3369(2)	10368(2)	4216(2)	41(1)
C(44)	4436(2)	11016(2)	3900(2)	42(1)
C(61)	5483(2)	7909(2)	3550(2)	31(1)
C(62)	6181(2)	8502(2)	3627(2)	46(1)
C(63)	5762(2)	7361(2)	4300(2)	42(1)
C(64)	5275(2)	7367(2)	2807(2)	38(1)
C(71)	4506(2)	5491(2)	3533(2)	30(1)
C(72)	5085(2)	4808(2)	3752(2)	30(1)
C(73)	5601(2)	4742(2)	3381(2)	38(1)
C(74)	6175(2)	4108(2)	3594(2)	46(1)
C(75)	6244(2)	3537(2)	4178(2)	51(1)
C(76)	5729(2)	3594(2)	4538(2)	51(1)
C(77)	5152(2)	4222(2)	4328(2)	42(1)
C(81)	1090(2)	9719(2)	2947(2)	32(1)
C(82)	461(2)	10255(2)	2970(2)	32(1)
C(83)	-331(2)	10192(2)	2383(2)	44(1)
C(84)	-934(2)	10710(2)	2405(2)	55(1)
C(85)	-754(2)	11277(2)	3015(2)	52(1)
C(86)	24(2)	11336(2)	3601(2)	56(1)
C(87)	632(2)	10831(2)	3579(2)	46(1)
C(90)	3072(3)	3461(3)	3017(3)	75(1)
C(91)	2698(2)	3624(2)	3582(2)	46(1)
C(92)	2168(2)	3052(2)	3661(2)	59(1)
C(93)	1815(3)	3200(3)	4165(3)	75(1)
C(94)	1983(3)	3922(3)	4606(3)	76(1)
C(95)	2514(2)	4495(3)	4547(2)	66(1)
C(96)	2862(2)	4357(2)	4032(2)	55(1)
C(100)	86(5)	2632(5)	1961(4)	168(4)
C(101)	476(3)	2856(4)	1538(3)	95(2)
C(102)	538(3)	3498(3)	1097(3)	79(1)
C(103)	907(10)	3730(9)	704(5)	310(11)
C(104)	1388(5)	2976(6)	789(5)	162(4)
C(105)	1504(3)	2228(4)	1204(4)	99(2)
C(106)	1061(3)	2103(4)	1607(3)	92(2)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 13. Bond Lengths [Å] and Angles [°] for **3**.

S(1)-Al(2)	2.1963(12)
S(1)-Al(1)	2.1977(11)
Al(1)-C(7)	1.911(3)
Al(1)-N(1)	1.938(2)
Al(1)-N(4)	1.963(2)
Al(1)-Al(2)	2.8086(13)
N(1)-C(1)	1.352(3)
N(1)-N(2)	1.410(3)
C(1)-C(2)	1.381(4)
C(1)-C(11)	1.516(4)
Al(2)-C(8)	1.903(3)
Al(2)-N(3)	1.940(2)
Al(2)-N(2)	1.958(2)
N(2)-C(3)	1.359(3)
C(2)-C(3)	1.382(4)
N(3)-C(4)	1.356(3)
N(3)-N(4)	1.408(3)
C(3)-C(31)	1.518(4)
N(4)-C(6)	1.351(3)
C(4)-C(5)	1.385(4)
C(4)-C(41)	1.517(4)
C(5)-C(6)	1.381(4)
C(6)-C(61)	1.527(4)
C(7)-C(71)	1.204(4)
C(8)-C(81)	1.206(4)
C(11)-C(14)	1.530(4)
C(11)-C(12)	1.535(4)
C(11)-C(13)	1.536(4)
C(31)-C(34)	1.525(4)
C(31)-C(33)	1.533(4)
C(31)-C(32)	1.537(4)
C(41)-C(43)	1.533(4)
C(41)-C(44)	1.537(4)
C(41)-C(42)	1.538(4)
C(61)-C(64)	1.532(4)
C(61)-C(63)	1.534(4)
C(61)-C(62)	1.539(4)
C(71)-C(72)	1.443(4)
C(72)-C(77)	1.384(4)
C(72)-C(73)	1.393(4)
C(73)-C(74)	1.381(4)
C(74)-C(75)	1.378(5)
C(75)-C(76)	1.374(5)
C(76)-C(77)	1.377(4)
C(81)-C(82)	1.443(4)
C(82)-C(87)	1.383(4)
C(82)-C(83)	1.390(4)
C(83)-C(84)	1.388(4)
C(84)-C(85)	1.372(5)
C(85)-C(86)	1.371(5)
C(86)-C(87)	1.383(4)
C(90)-C(91)	1.507(5)
C(91)-C(92)	1.378(5)
C(91)-C(96)	1.386(5)
C(92)-C(93)	1.372(5)
C(93)-C(94)	1.363(6)
C(94)-C(95)	1.366(6)
C(95)-C(96)	1.379(5)
C(100)-C(101)	1.318(8)
C(101)-C(102)	1.343(7)
C(101)-C(106)	1.568(8)
C(102)-C(103)	1.246(10)
C(103)-C(104)	1.45(2)
C(104)-C(105)	1.381(10)
C(105)-C(106)	1.335(8)
Al(2)-S(1)-Al(1)	79.46(4)
C(7)-Al(1)-N(1)	118.15(11)
C(7)-Al(1)-N(4)	115.49(11)
N(1)-Al(1)-N(4)	98.65(10)
C(7)-Al(1)-S(1)	119.80(10)
N(1)-Al(1)-S(1)	100.18(7)
N(4)-Al(1)-S(1)	101.01(7)
C(7)-Al(1)-Al(2)	169.75(10)
N(1)-Al(1)-Al(2)	69.38(7)
N(4)-Al(1)-Al(2)	68.06(7)
S(1)-Al(1)-Al(2)	50.25(3)
C(1)-N(1)-N(2)	107.6(2)
C(1)-N(1)-Al(1)	142.0(2)
N(2)-N(1)-Al(1)	110.3(2)

N(1)-C(1)-C(2)	108.7(2)
N(1)-C(1)-C(11)	124.8(2)
C(2)-C(1)-C(11)	126.4(2)
C(8)-Al(2)-N(3)	119.13(11)
C(8)-Al(2)-N(2)	116.42(11)
N(3)-Al(2)-N(2)	97.73(9)
C(8)-Al(2)-S(1)	117.77(10)
N(3)-Al(2)-S(1)	99.90(7)
N(2)-Al(2)-S(1)	102.47(8)
C(8)-Al(2)-Al(1)	167.71(9)
N(3)-Al(2)-Al(1)	69.71(7)
N(2)-Al(2)-Al(1)	68.22(7)
S(1)-Al(2)-Al(1)	50.29(3)
C(3)-N(2)-N(1)	107.6(2)
C(3)-N(2)-Al(2)	140.4(2)
N(1)-N(2)-Al(2)	111.1(2)
C(1)-C(2)-C(3)	107.6(2)
C(4)-N(3)-N(4)	107.9(2)
C(4)-N(3)-Al(2)	142.0(2)
N(4)-N(3)-Al(2)	110.1(2)
N(2)-C(3)-C(2)	108.4(2)
N(2)-C(3)-C(31)	125.5(2)
C(2)-C(3)-C(31)	126.0(2)
C(6)-N(4)-N(3)	107.5(2)
C(6)-N(4)-Al(1)	140.3(2)
N(3)-N(4)-Al(1)	111.6(2)
N(3)-C(4)-C(5)	108.2(2)
N(3)-C(4)-C(41)	124.7(2)
C(5)-C(4)-C(41)	127.0(2)
C(6)-C(5)-C(4)	107.5(2)
N(4)-C(6)-C(5)	108.9(2)
N(4)-C(6)-C(61)	125.2(2)
C(5)-C(6)-C(61)	125.9(2)
C(71)-C(7)-Al(1)	175.9(2)
C(81)-C(8)-Al(2)	174.3(3)
C(1)-C(11)-C(14)	109.4(2)
C(1)-C(11)-C(12)	110.9(2)
C(14)-C(11)-C(12)	108.0(2)
C(1)-C(11)-C(13)	109.5(2)
C(14)-C(11)-C(13)	108.5(3)
C(12)-C(11)-C(13)	110.4(2)
C(3)-C(31)-C(34)	111.6(2)
C(3)-C(31)-C(33)	109.1(2)
C(34)-C(31)-C(33)	110.4(2)
C(3)-C(31)-C(32)	108.7(2)
C(34)-C(31)-C(32)	107.9(2)
C(33)-C(31)-C(32)	109.0(3)
C(4)-C(41)-C(43)	109.9(2)
C(4)-C(41)-C(44)	109.4(2)
C(43)-C(41)-C(44)	108.3(2)
C(4)-C(41)-C(42)	110.9(2)
C(43)-C(41)-C(42)	110.1(2)
C(44)-C(41)-C(42)	108.1(2)
C(6)-C(61)-C(64)	110.7(2)
C(6)-C(61)-C(63)	109.9(2)
C(64)-C(61)-C(63)	111.3(2)
C(6)-C(61)-C(62)	108.6(2)
C(64)-C(61)-C(62)	107.3(2)
C(63)-C(61)-C(62)	108.9(2)
C(7)-C(71)-C(72)	176.0(3)
C(77)-C(72)-C(73)	118.9(3)
C(77)-C(72)-C(71)	122.0(3)
C(73)-C(72)-C(71)	119.0(3)
C(74)-C(73)-C(72)	120.2(3)
C(75)-C(74)-C(73)	120.2(3)
C(76)-C(75)-C(74)	119.7(3)
C(75)-C(76)-C(77)	120.7(3)
C(76)-C(77)-C(72)	120.3(3)
C(8)-C(81)-C(82)	179.5(3)
C(87)-C(82)-C(83)	118.9(3)
C(87)-C(82)-C(81)	120.8(3)
C(83)-C(82)-C(81)	120.4(3)
C(84)-C(83)-C(82)	120.2(3)
C(85)-C(84)-C(83)	120.1(3)
C(86)-C(85)-C(84)	120.0(3)
C(85)-C(86)-C(87)	120.3(3)
C(86)-C(87)-C(82)	120.4(3)
C(92)-C(91)-C(96)	117.6(3)
C(92)-C(91)-C(90)	120.9(3)
C(96)-C(91)-C(90)	121.5(3)
C(93)-C(92)-C(91)	121.4(4)
C(94)-C(93)-C(92)	120.4(4)
C(93)-C(94)-C(95)	119.4(4)

C(94)-C(95)-C(96)	120.5(4)
C(95)-C(96)-C(91)	120.7(4)
C(100)-C(101)-C(102)	141.2(8)
C(100)-C(101)-C(106)	105.8(7)
C(102)-C(101)-C(106)	113.0(5)
C(103)-C(102)-C(101)	142.5(11)
C(102)-C(103)-C(104)	98.7(10)
C(105)-C(104)-C(103)	134.9(11)
C(106)-C(105)-C(104)	117.3(7)
C(105)-C(106)-C(101)	113.5(6)

Symmetry transformations used to generate equivalent atoms: #1 x+1,y,-z+1/2

Table 14. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**.

	U11	U22	U33	U23	U13	U12
S(1)	29(1)	30(1)	37(1)	8(1)	18(1)	4(1)
Al(1)	21(1)	21(1)	32(1)	2(1)	10(1)	3(1)
N(1)	20(1)	21(1)	33(1)	1(1)	10(1)	5(1)
C(1)	23(1)	28(1)	33(2)	-2(1)	14(1)	-1(1)
Al(2)	20(1)	24(1)	30(1)	1(1)	12(1)	3(1)
N(2)	21(1)	21(1)	31(1)	2(1)	10(1)	4(1)
C(2)	29(1)	30(2)	29(1)	-3(1)	8(1)	0(1)
N(3)	23(1)	21(1)	30(1)	-1(1)	11(1)	4(1)
C(3)	21(1)	28(1)	29(1)	1(1)	7(1)	-1(1)
N(4)	20(1)	22(1)	33(1)	-1(1)	10(1)	4(1)
C(4)	25(1)	26(1)	25(1)	-1(1)	9(1)	-1(1)
C(5)	23(1)	29(2)	34(2)	-6(1)	12(1)	-4(1)
C(6)	21(1)	28(1)	29(1)	-1(1)	11(1)	-1(1)
C(7)	28(1)	27(2)	38(2)	3(1)	13(1)	3(1)
C(8)	26(1)	32(2)	35(2)	0(1)	13(1)	5(1)
C(11)	29(1)	27(2)	40(2)	-9(1)	15(1)	1(1)
C(12)	35(2)	37(2)	58(2)	-5(2)	25(2)	6(1)
C(13)	40(2)	27(2)	56(2)	-5(1)	22(2)	-1(1)
C(14)	47(2)	44(2)	49(2)	-17(2)	16(2)	6(2)
C(31)	32(2)	26(1)	32(2)	1(1)	6(1)	3(1)
C(32)	63(2)	38(2)	35(2)	5(2)	4(2)	10(2)
C(33)	27(2)	37(2)	70(2)	6(2)	12(2)	6(1)
C(34)	39(2)	27(2)	39(2)	6(1)	11(1)	3(1)
C(41)	28(1)	25(1)	33(2)	-4(1)	9(1)	1(1)
C(42)	38(2)	30(2)	42(2)	2(1)	11(1)	3(1)
C(43)	42(2)	39(2)	41(2)	-10(1)	19(1)	-1(1)
C(44)	37(2)	29(2)	54(2)	-9(1)	16(2)	-3(1)
C(61)	21(1)	32(2)	41(2)	-4(1)	14(1)	1(1)
C(62)	26(2)	47(2)	69(2)	-15(2)	24(2)	-5(1)
C(63)	30(2)	43(2)	45(2)	-1(2)	8(1)	9(1)
C(64)	32(2)	38(2)	48(2)	-8(1)	21(1)	1(1)
C(71)	28(1)	27(2)	34(2)	4(1)	11(1)	3(1)
C(72)	28(1)	26(1)	30(1)	1(1)	8(1)	6(1)
C(73)	36(2)	39(2)	41(2)	0(1)	17(1)	5(1)
C(74)	37(2)	50(2)	53(2)	-12(2)	20(2)	8(2)
C(75)	42(2)	41(2)	54(2)	-7(2)	7(2)	22(2)
C(76)	64(2)	38(2)	43(2)	13(2)	15(2)	21(2)
C(77)	47(2)	36(2)	46(2)	9(1)	22(2)	14(1)
C(81)	30(2)	32(2)	36(2)	4(1)	15(1)	3(1)
C(82)	29(1)	30(2)	42(2)	4(1)	20(1)	7(1)
C(83)	32(2)	47(2)	50(2)	-7(2)	15(2)	8(1)
C(84)	28(2)	62(2)	68(2)	2(2)	16(2)	13(2)
C(85)	43(2)	53(2)	71(2)	10(2)	34(2)	25(2)
C(86)	64(2)	51(2)	57(2)	-6(2)	30(2)	23(2)
C(87)	37(2)	48(2)	48(2)	-6(2)	14(2)	16(2)
C(90)	96(3)	72(3)	73(3)	-9(2)	51(3)	-12(3)
C(91)	47(2)	45(2)	43(2)	1(2)	18(2)	0(2)
C(92)	58(2)	53(2)	68(2)	-17(2)	28(2)	-16(2)
C(93)	70(3)	79(3)	93(3)	-17(3)	51(3)	-23(2)
C(94)	69(3)	91(3)	85(3)	-22(3)	49(3)	-7(3)
C(95)	61(2)	61(3)	74(3)	-26(2)	28(2)	-3(2)
C(96)	52(2)	45(2)	63(2)	-2(2)	21(2)	-6(2)
C(100)	166(7)	190(8)	96(5)	11(5)	9(5)	-92(6)
C(101)	112(4)	119(5)	58(3)	-36(3)	40(3)	-71(4)
C(102)	78(3)	50(2)	73(3)	2(2)	-2(2)	-5(2)
C(103)	461(21)	377(17)	66(4)	-73(8)	90(9)	-378(18)
C(104)	138(6)	157(8)	110(6)	-55(6)	-22(5)	-45(7)
C(105)	65(3)	110(5)	85(4)	-39(3)	-4(3)	23(3)
C(106)	60(3)	102(4)	88(4)	-50(3)	7(3)	10(3)

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h^2 a*^2 U11 + ... + 2 h k a* b* U12].

Table 15. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters ($Å^2$ x 10^3) for **3**.

	x	y	z	U(eq)
H(2A)	1521(2)	7322(2)	138(2)	37
H(5A)	5229(2)	9654(2)	3798(2)	34
H(12A)	3694(4)	5504(5)	1119(12)	63
H(12B)	3866(2)	6162(14)	1812(3)	63
H(12C)	3639(3)	6485(9)	938(10)	63
H(13A)	2625(12)	4813(2)	1453(9)	61
H(13B)	1901(3)	5364(9)	1453(9)	61
H(13C)	2791(10)	5486(8)	2134(2)	61
H(14A)	2319(10)	5268(7)	88(4)	73
H(14B)	2250(11)	6240(8)	-132(2)	73
H(14C)	1578(2)	5806(15)	66(4)	73
H(32A)	521(12)	9341(9)	-401(3)	77
H(32B)	604(13)	8346(7)	-410(3)	77
H(32C)	1364(3)	8927(15)	-252(2)	77
H(33A)	-11(7)	9166(7)	650(13)	71
H(33B)	508(2)	8638(15)	1427(2)	71
H(33C)	89(8)	8178(8)	593(12)	71
H(34A)	1141(5)	10138(2)	805(8)	56
H(34B)	2013(6)	9747(6)	1036(11)	56
H(34C)	1619(11)	9701(5)	1644(3)	56
H(42A)	2926(9)	11330(5)	2884(3)	59
H(42B)	2581(5)	10405(8)	2626(7)	59
H(42C)	3275(5)	10752(12)	2411(4)	59
H(43A)	3204(12)	10929(3)	4296(9)	61
H(43B)	3784(4)	10158(13)	4715(4)	61
H(43C)	2904(8)	9993(10)	4030(6)	61
H(44A)	4255(3)	11576(4)	3962(12)	62
H(44B)	4669(8)	11038(10)	3522(6)	62
H(44C)	4843(6)	10820(8)	4410(6)	62
H(62A)	6638(5)	8170(2)	3653(14)	69
H(62B)	6346(9)	8836(10)	4107(7)	69
H(62C)	5999(5)	8874(10)	3169(7)	69
H(63A)	6225(8)	7023(10)	4351(7)	63
H(63B)	5322(5)	6993(10)	4261(6)	63
H(63C)	5916(12)	7722(2)	4763(2)	63
H(64A)	5754(4)	7058(10)	2858(6)	57
H(64B)	5092(12)	7728(2)	2342(2)	57
H(64C)	4848(9)	6972(9)	2750(7)	57
H(73A)	5557(2)	5130(2)	2984(2)	46
H(74A)	6520(2)	4065(2)	3341(2)	55
H(75A)	6641(2)	3111(2)	4329(2)	61
H(76A)	5772(2)	3201(2)	4932(2)	61
H(77A)	4801(2)	4252(2)	4576(2)	51
H(83A)	-459(2)	9798(2)	1969(2)	53
H(84A)	-1467(2)	10672(2)	2003(2)	65
H(85A)	-1164(2)	11625(2)	3030(2)	63
H(86A)	145(2)	11722(2)	4020(2)	67
H(87A)	1164(2)	10879(2)	3981(2)	55
H(90A)	3277(17)	3987(4)	2907(14)	112
H(90B)	2666(6)	3229(18)	2525(7)	112
H(90C)	3516(12)	3063(15)	3255(8)	112
H(92A)	2047(2)	2551(2)	3363(2)	71
H(93A)	1454(3)	2801(3)	4208(3)	90
H(94A)	1736(3)	4025(3)	4947(3)	91
H(95A)	2643(2)	4986(3)	4860(2)	79
H(96A)	3214(2)	4763(2)	3986(2)	66
H(10A)	191(33)	2041(13)	2106(34)	251
H(10B)	-492(6)	2717(41)	1648(16)	251
H(10C)	272(31)	2974(30)	2438(21)	251
H(10D)	171(3)	3924(3)	1077(3)	95
H(10E)	881(10)	4239(9)	435(5)	372
H(10F)	1693(5)	3003(6)	492(5)	194
H(10G)	1880(3)	1822(4)	1204(4)	119
H(10I)	1096(3)	1612(4)	1902(3)	111

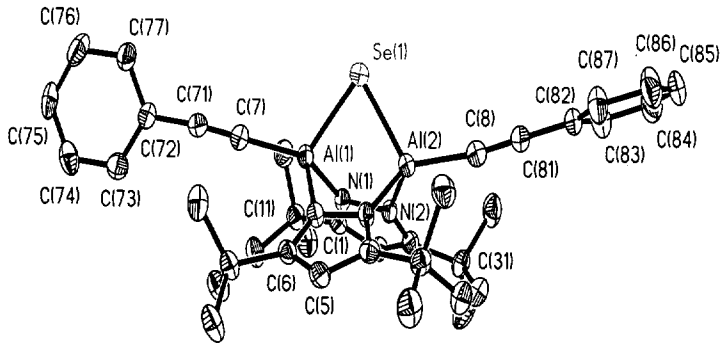

Figure 4. Ortep plot of [(η^1-η^1-3,5-*t*Bupz)$_2$(μ-Se)(μ-Al)(C≡CPh)$_2$] (**7**).

Table 16. Crystal Data and Structure Refinement for **7**.

Empirical formula	C52 H64 Al2 N4 Se
Formula weight	877.99
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 18.291(3) A alpha = 90 deg. b = 15.891(6) A beta = 115.261(11) deg. c = 18.594(3) A gamma = 90 deg.
Volume, Z	4888(2) A^3, 4
Density (calculated)	1.193 Mg/m^3
Absorption coefficient	0.842 mm^-1
F(000)	1856
Crystal size	0.70 x 0.20 x 0.20 mm
Theta range for data collection	3.53 to 25.05 deg.
Limiting indices	-21<=h<=21, -18<=k<=18, -22<=l<=22
Reflections collected	12675
Independent reflections	8620 [R(int) = 0.0553]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8583 / 15 / 546
Goodness-of-fit on F^2	1.089
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.0992
R indices (all data)	R1 = 0.0813, wR2 = 0.1221
Largest diff. peak and hole	0.824 and -0.750 e.A^-3

Table 17. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for **7**.

	x	y	z	U(eq)
Se(1)	2582(1)	7333(1)	3717(1)	31(1)
Al(1)	3405(1)	7095(1)	3067(1)	25(1)
N(1)	2640(2)	7265(2)	1970(2)	24(1)
C(1)	2372(2)	6898(2)	1240(2)	26(1)
Al(2)	2392(1)	8506(1)	2909(1)	24(1)
N(2)	2214(2)	8023(2)	1881(2)	24(1)
C(2)	1802(2)	7419(2)	693(2)	30(1)
N(3)	3505(2)	8856(2)	3233(2)	24(1)
C(3)	1710(2)	8108(2)	1093(2)	27(1)
N(4)	3987(2)	8164(2)	3234(2)	26(1)
C(4)	3988(2)	9541(2)	3476(2)	26(1)
C(5)	4763(2)	9304(2)	3623(2)	29(1)
C(6)	4749(2)	8455(2)	3464(2)	26(1)
C(7)	4063(2)	6112(2)	3324(2)	32(1)
C(8)	1620(2)	9312(2)	2907(2)	32(1)
C(11)	2640(2)	6040(2)	1082(2)	32(1)
C(12)	3534(2)	6059(3)	1238(3)	40(1)
C(13)	2489(2)	5372(2)	1596(2)	39(1)
C(14)	2137(3)	5811(3)	205(2)	44(1)
C(31)	1131(2)	8835(2)	729(2)	32(1)
C(32)	891(3)	8846(3)	-169(2)	53(1)
C(33)	373(2)	8701(3)	874(3)	48(1)
C(34)	1520(2)	9682(2)	1069(2)	38(1)
C(41)	3710(2)	10410(2)	3594(2)	30(1)
C(42)	3070(2)	10759(2)	2807(2)	38(1)
C(43)	3365(2)	10371(3)	4216(2)	40(1)
C(44)	4433(2)	11016(2)	3892(3)	44(1)
C(61)	5474(2)	7920(2)	3547(2)	33(1)
C(62)	6171(2)	8509(3)	3628(3)	45(1)
C(63)	5751(2)	7371(3)	4297(2)	42(1)
C(64)	5274(2)	7380(3)	2801(2)	39(1)
C(71)	4509(2)	5510(2)	3524(2)	30(1)
C(72)	5081(2)	4830(2)	3736(2)	30(1)
C(73)	5604(2)	4765(3)	3375(2)	38(1)
C(74)	6171(2)	4124(3)	3583(3)	44(1)
C(75)	6220(3)	3550(3)	4154(3)	47(1)
C(76)	5694(3)	3601(3)	4507(3)	49(1)
C(77)	5132(2)	4230(3)	4309(2)	40(1)
C(81)	1100(2)	9750(2)	2943(2)	32(1)
C(82)	474(2)	10274(2)	2975(2)	33(1)
C(83)	-317(2)	10204(3)	2399(3)	45(1)
C(84)	-917(3)	10712(3)	2435(3)	54(1)
C(85)	-735(3)	11277(3)	3038(3)	51(1)
C(86)	39(3)	11352(3)	3617(3)	57(1)
C(87)	646(3)	10850(3)	3589(3)	47(1)
C(91)	2699(3)	11372(3)	-1429(3)	47(1)
C(92)	2173(3)	11945(3)	-1347(3)	62(1)
C(93)	1819(3)	11792(4)	-840(4)	80(2)
C(94)	1987(4)	11061(4)	-416(4)	81(2)
C(95)	2512(3)	10486(4)	-473(3)	71(2)
C(96)	2857(3)	10638(3)	-984(3)	56(1)
C(90)	3077(4)	11534(4)	-1992(3)	74(2)
C(101)	-481(4)	7147(5)	-1550(4)	98(2)
C(102)	-1048(4)	7894(4)	-1600(4)	90(2)
C(103)	-1498(4)	7773(6)	-1207(5)	101(2)
C(104)	-1416(7)	7033(8)	-783(7)	180(6)
C(105)	-965(9)	6314(9)	-729(6)	319(15)
C(106)	-550(4)	6492(4)	-1111(3)	74(2)
C(107)	-63(5)	7325(6)	-1974(5)	164(4)

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table 18. Bond Lengths [Å] and Angles [°] for **7**.

Se(1)-Al(2)	2.3258(13)
Se(1)-Al(1)	2.3293(11)
Al(1)-C(7)	1.905(4)
Al(1)-N(1)	1.938(3)
Al(1)-N(4)	1.958(3)
Al(1)-Al(2)	2.843(2)
N(1)-C(1)	1.361(4)
N(1)-N(2)	1.406(4)
C(1)-C(2)	1.379(5)
C(1)-C(11)	1.519(5)
Al(2)-C(8)	1.905(4)
Al(2)-N(3)	1.941(3)
Al(2)-N(2)	1.954(3)
N(2)-C(3)	1.364(4)
C(2)-C(3)	1.373(5)
N(3)-C(4)	1.353(4)
N(3)-N(4)	1.408(4)
C(3)-C(31)	1.517(5)
N(4)-C(6)	1.354(4)
C(4)-C(5)	1.378(5)
C(4)-C(41)	1.520(5)
C(5)-C(6)	1.379(5)
C(6)-C(61)	1.527(5)
C(7)-C(71)	1.209(5)
C(8)-C(81)	1.204(5)
C(11)-C(13)	1.530(5)
C(11)-C(12)	1.535(5)
C(11)-C(14)	1.536(5)
C(31)-C(34)	1.527(5)
C(31)-C(33)	1.536(5)
C(31)-C(32)	1.536(5)
C(41)-C(42)	1.535(5)
C(41)-C(44)	1.535(5)
C(41)-C(43)	1.538(5)
C(61)-C(62)	1.535(5)
C(61)-C(63)	1.536(5)
C(61)-C(64)	1.538(5)
C(71)-C(72)	1.437(5)
C(72)-C(73)	1.389(5)
C(72)-C(77)	1.402(5)
C(73)-C(74)	1.386(5)
C(74)-C(75)	1.373(6)
C(75)-C(76)	1.378(6)
C(76)-C(77)	1.368(5)
C(81)-C(82)	1.438(5)
C(82)-C(83)	1.389(5)
C(82)-C(87)	1.392(6)
C(83)-C(84)	1.386(6)
C(84)-C(85)	1.362(6)
C(85)-C(86)	1.371(6)
C(86)-C(87)	1.385(6)
C(91)-C(92)	1.380(6)
C(91)-C(96)	1.387(6)
C(91)-C(90)	1.503(6)
C(92)-C(93)	1.374(7)
C(93)-C(94)	1.363(7)
C(94)-C(95)	1.362(7)
C(95)-C(96)	1.368(6)
C(101)-C(107)	1.343(9)
C(101)-C(106)	1.361(8)
C(101)-C(102)	1.552(9)
C(102)-C(103)	1.327(9)
C(103)-C(104)	1.387(12)
C(104)-C(105)	1.39(2)
C(105)-C(106)	1.274(11)
Al(2)-Se(1)-Al(1)	75.28(4)
C(7)-Al(1)-N(1)	118.2(2)
C(7)-Al(1)-N(4)	115.44(14)
N(1)-Al(1)-N(4)	98.38(13)
C(7)-Al(1)-Se(1)	118.84(12)
N(1)-Al(1)-Se(1)	100.81(9)
N(4)-Al(1)-Se(1)	101.81(9)
C(7)-Al(1)-Al(2)	170.82(12)
N(1)-Al(1)-Al(2)	68.63(9)
N(4)-Al(1)-Al(2)	67.54(9)
Se(1)-Al(1)-Al(2)	52.31(3)
C(1)-N(1)-N(2)	107.7(3)
C(1)-N(1)-Al(1)	141.3(2)

N(2)-N(1)-Al(1)	111.0(2)
N(1)-C(1)-C(2)	108.4(3)
N(1)-C(1)-C(11)	124.6(3)
C(2)-C(1)-C(11)	127.0(3)
C(8)-Al(2)-N(3)	119.1(2)
C(8)-Al(2)-N(2)	116.6(2)
N(3)-Al(2)-N(2)	97.51(12)
C(8)-Al(2)-Se(1)	116.54(12)
N(3)-Al(2)-Se(1)	100.45(9)
N(2)-Al(2)-Se(1)	103.55(9)
C(8)-Al(2)-Al(1)	168.62(12)
N(3)-Al(2)-Al(1)	69.08(9)
N(2)-Al(2)-Al(1)	67.71(9)
Se(1)-Al(2)-Al(1)	52.41(3)
C(3)-N(2)-N(1)	107.3(3)
C(3)-N(2)-Al(2)	140.0(2)
N(1)-N(2)-Al(2)	111.6(2)
C(3)-C(2)-C(1)	107.9(3)
C(4)-N(3)-N(4)	108.0(3)
C(4)-N(3)-Al(2)	141.5(2)
N(4)-N(3)-Al(2)	110.5(2)
N(2)-C(3)-C(2)	108.7(3)
N(2)-C(3)-C(31)	125.2(3)
C(2)-C(3)-C(31)	126.1(3)
C(6)-N(4)-N(3)	107.1(3)
C(6)-N(4)-Al(1)	139.8(2)
N(3)-N(4)-Al(1)	112.3(2)
N(3)-C(4)-C(5)	108.4(3)
N(3)-C(4)-C(41)	124.7(3)
C(5)-C(4)-C(41)	126.8(3)
C(4)-C(5)-C(6)	107.5(3)
N(4)-C(6)-C(5)	108.9(3)
N(4)-C(6)-C(61)	125.1(3)
C(5)-C(6)-C(61)	125.9(3)
C(71)-C(7)-Al(1)	176.5(3)
C(81)-C(8)-Al(2)	172.4(3)
C(1)-C(11)-C(13)	110.1(3)
C(1)-C(11)-C(12)	110.5(3)
C(13)-C(11)-C(12)	111.0(3)
C(1)-C(11)-C(14)	108.8(3)
C(13)-C(11)-C(14)	108.2(3)
C(12)-C(11)-C(14)	108.2(3)
C(3)-C(31)-C(34)	111.9(3)
C(3)-C(31)-C(33)	109.1(3)
C(34)-C(31)-C(33)	110.2(3)
C(3)-C(31)-C(32)	108.4(3)
C(34)-C(31)-C(32)	107.8(3)
C(33)-C(31)-C(32)	109.3(3)
C(4)-C(41)-C(42)	110.9(3)
C(4)-C(41)-C(44)	109.4(3)
C(42)-C(41)-C(44)	107.9(3)
C(4)-C(41)-C(43)	109.9(3)
C(42)-C(41)-C(43)	109.9(3)
C(44)-C(41)-C(43)	108.8(3)
C(6)-C(61)-C(62)	108.6(3)
C(6)-C(61)-C(63)	110.1(3)
C(62)-C(61)-C(63)	108.6(3)
C(6)-C(61)-C(64)	111.0(3)
C(62)-C(61)-C(64)	107.3(3)
C(63)-C(61)-C(64)	111.2(3)
C(7)-C(71)-C(72)	175.3(4)
C(73)-C(72)-C(77)	118.8(3)
C(73)-C(72)-C(71)	119.5(3)
C(77)-C(72)-C(71)	121.6(3)
C(74)-C(73)-C(72)	120.4(4)
C(75)-C(74)-C(73)	119.9(4)
C(74)-C(75)-C(76)	120.1(4)
C(77)-C(76)-C(75)	120.8(4)
C(76)-C(77)-C(72)	120.0(4)
C(8)-C(81)-C(82)	179.1(4)
C(83)-C(82)-C(87)	118.8(4)
C(83)-C(82)-C(81)	120.6(4)
C(87)-C(82)-C(81)	120.6(4)
C(84)-C(83)-C(82)	120.1(4)
C(85)-C(84)-C(83)	120.2(4)
C(84)-C(85)-C(86)	120.8(4)
C(85)-C(86)-C(87)	119.7(4)
C(86)-C(87)-C(82)	120.4(4)
C(92)-C(91)-C(96)	117.9(4)
C(92)-C(91)-C(90)	120.9(4)
C(96)-C(91)-C(90)	121.3(4)
C(93)-C(92)-C(91)	120.9(5)
C(94)-C(93)-C(92)	119.5(5)

C(95)-C(94)-C(93)	121.3(5)
C(94)-C(95)-C(96)	119.0(5)
C(95)-C(96)-C(91)	121.5(5)
C(107)-C(101)-C(106)	137.3(9)
C(107)-C(101)-C(102)	109.7(8)
C(106)-C(101)-C(102)	113.0(6)
C(103)-C(102)-C(101)	114.3(7)
C(102)-C(103)-C(104)	119.5(8)
C(105)-C(104)-C(103)	131.0(13)
C(106)-C(105)-C(104)	104.7(11)
C(105)-C(106)-C(101)	137.2(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Table 19. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **7**.

	U11	U22	U33	U23	U13	U12
Se(1)	31(1)	33(1)	33(1)	7(1)	18(1)	4(1)
Al(1)	22(1)	24(1)	29(1)	2(1)	10(1)	3(1)
N(1)	23(1)	22(2)	28(2)	0(1)	11(1)	3(1)
C(1)	23(2)	28(2)	31(2)	-3(2)	14(2)	-3(2)
Al(2)	21(1)	26(1)	27(1)	1(1)	12(1)	3(1)
N(2)	22(2)	23(2)	28(2)	3(1)	10(1)	4(1)
C(2)	31(2)	31(2)	26(2)	0(2)	11(2)	3(2)
N(3)	23(2)	21(2)	30(2)	-1(1)	12(1)	4(1)
C(3)	21(2)	29(2)	31(2)	4(2)	10(2)	1(2)
N(4)	21(2)	26(2)	29(2)	-1(1)	11(1)	2(1)
C(4)	27(2)	29(2)	20(2)	0(2)	10(2)	-1(2)
C(5)	25(2)	31(2)	30(2)	-4(2)	11(2)	-3(2)
C(6)	20(2)	32(2)	24(2)	1(2)	9(2)	1(2)
C(7)	30(2)	32(2)	33(2)	6(2)	13(2)	5(2)
C(8)	31(2)	32(2)	34(2)	1(2)	16(2)	2(2)
C(11)	33(2)	27(2)	37(2)	-4(2)	16(2)	1(2)
C(12)	34(2)	36(2)	54(3)	-7(2)	21(2)	5(2)
C(13)	43(2)	28(2)	47(2)	-2(2)	21(2)	3(2)
C(14)	48(3)	41(2)	43(3)	-13(2)	19(2)	5(2)
C(31)	29(2)	31(2)	28(2)	3(2)	3(2)	5(2)
C(32)	72(3)	41(3)	27(2)	2(2)	2(2)	14(2)
C(33)	27(2)	40(3)	68(3)	5(2)	12(2)	5(2)
C(34)	41(2)	30(2)	38(2)	4(2)	13(2)	4(2)
C(41)	33(2)	22(2)	34(2)	-3(2)	14(2)	-1(2)
C(42)	39(2)	29(2)	42(2)	0(2)	13(2)	4(2)
C(43)	44(2)	40(2)	39(2)	-8(2)	20(2)	4(2)
C(44)	40(2)	31(2)	57(3)	-10(2)	18(2)	-4(2)
C(61)	23(2)	35(2)	40(2)	-5(2)	14(2)	0(2)
C(62)	26(2)	50(3)	62(3)	-11(2)	21(2)	-1(2)
C(63)	35(2)	44(2)	41(2)	-1(2)	10(2)	10(2)
C(64)	35(2)	42(2)	45(2)	-11(2)	21(2)	0(2)
C(71)	32(2)	31(2)	30(2)	3(2)	15(2)	2(2)
C(72)	31(2)	28(2)	26(2)	0(2)	8(2)	6(2)
C(73)	41(2)	41(2)	34(2)	2(2)	18(2)	4(2)
C(74)	36(2)	51(3)	45(3)	-10(2)	19(2)	10(2)
C(75)	41(2)	43(3)	43(3)	-3(2)	7(2)	24(2)
C(76)	64(3)	36(2)	43(3)	12(2)	18(2)	21(2)
C(77)	47(2)	39(2)	39(2)	9(2)	22(2)	16(2)
C(81)	32(2)	32(2)	34(2)	4(2)	17(2)	7(2)
C(82)	31(2)	32(2)	42(2)	6(2)	20(2)	9(2)
C(83)	35(2)	45(3)	55(3)	-7(2)	19(2)	7(2)
C(84)	33(2)	60(3)	67(3)	5(3)	18(2)	14(2)
C(85)	47(3)	52(3)	69(3)	9(2)	37(3)	24(2)
C(86)	62(3)	60(3)	55(3)	-9(2)	31(3)	23(3)
C(87)	42(2)	50(3)	47(3)	-5(2)	16(2)	17(2)
C(91)	47(3)	50(3)	42(3)	2(2)	16(2)	1(2)
C(92)	65(3)	59(3)	66(3)	19(3)	32(3)	18(3)
C(93)	81(4)	83(4)	94(5)	21(4)	55(4)	30(3)
C(94)	80(4)	96(5)	88(4)	31(4)	55(4)	12(4)
C(95)	70(4)	66(4)	81(4)	30(3)	37(3)	6(3)
C(96)	53(3)	49(3)	64(3)	5(2)	24(3)	3(2)
C(90)	99(4)	76(4)	67(4)	9(3)	52(3)	14(3)
C(101)	108(5)	131(6)	60(4)	-44(4)	41(4)	-66(5)
C(102)	62(4)	106(5)	78(4)	-49(4)	5(3)	6(4)
C(103)	66(4)	119(7)	84(5)	-33(5)	1(4)	15(4)
C(104)	167(10)	179(13)	108(9)	-52(9)	-23(7)	-61(10)
C(105)	469(28)	407(24)	64(6)	-82(11)	98(12)	-391(23)
C(106)	82(4)	52(3)	67(4)	0(3)	10(3)	-8(3)
C(107)	164(8)	202(10)	98(6)	2(6)	29(6)	-99(8)

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$.

Table 20. Hydrogen Coordinates (x 10^4) and Isotropic Displacement Parameters (Å^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(2A)	1526(2)	7321(2)	144(2)	36
H(5A)	5219(2)	9657(2)	3800(2)	34
H(12A)	3686(5)	5517(6)	1106(15)	61
H(12B)	3864(3)	6182(17)	1795(4)	61
H(12C)	3616(4)	6492(12)	911(12)	61
H(13A)	2632(15)	4822(3)	1469(11)	58
H(13B)	1922(4)	5376(11)	1493(11)	58
H(13C)	2817(12)	5495(9)	2154(2)	58
H(14A)	2291(12)	5256(8)	102(5)	66
H(14B)	2234(13)	6220(10)	-131(2)	66
H(14C)	1567(3)	5811(17)	90(5)	66
H(32A)	548(15)	9329(11)	-406(4)	80
H(32B)	599(16)	8334(9)	-407(4)	80
H(32C)	1373(3)	8882(19)	-261(2)	80
H(33A)	5(8)	9170(9)	652(16)	71
H(33B)	526(3)	8665(19)	1441(3)	71
H(33C)	107(10)	8183(10)	619(15)	71
H(34A)	1146(6)	10132(2)	796(11)	57
H(34B)	2010(9)	9749(7)	994(14)	57
H(34C)	1651(14)	9702(7)	1632(4)	57
H(42A)	2931(12)	11329(6)	2888(4)	57
H(42B)	2591(6)	10409(10)	2625(8)	57
H(42C)	3284(6)	10760(15)	2412(5)	57
H(43A)	3194(14)	10928(4)	4292(11)	60
H(43B)	3777(5)	10167(16)	4716(5)	60
H(43C)	2905(10)	9992(13)	4032(7)	60
H(44A)	4254(4)	11574(5)	3957(16)	65
H(44B)	4663(10)	11038(13)	3509(8)	65
H(44C)	4840(8)	10819(10)	4399(8)	65
H(62A)	6621(7)	8178(3)	3637(17)	68
H(62B)	6343(11)	8828(13)	4118(9)	68
H(62C)	5989(5)	8893(12)	3180(9)	68
H(63A)	6216(10)	7041(13)	4349(9)	63
H(63B)	5315(6)	6998(12)	4255(7)	63
H(63C)	5895(15)	7729(3)	4760(3)	63
H(64A)	5753(5)	7074(12)	2852(7)	59
H(64B)	5094(15)	7740(3)	2336(3)	59
H(64C)	4849(11)	6984(11)	2743(9)	59
H(73A)	5574(2)	5160(3)	2986(2)	45
H(74A)	6522(2)	4082(3)	3334(3)	52
H(75A)	6611(3)	3121(3)	4304(3)	56
H(76A)	5724(3)	3199(3)	4889(3)	59
H(77A)	4779(2)	4260(3)	4557(2)	48
H(83A)	-446(2)	9811(3)	1985(3)	54
H(84A)	-1451(3)	10667(3)	2041(3)	65
H(85A)	-1145(3)	11619(3)	3056(3)	62
H(86A)	158(3)	11741(3)	4033(3)	68
H(87A)	1177(3)	10900(3)	3987(3)	57
H(92A)	2055(3)	12447(3)	-1642(3)	74
H(93A)	1463(3)	12187(4)	-786(4)	96
H(94A)	1737(4)	10952(4)	-77(4)	97
H(95A)	2635(3)	9991(4)	-166(3)	85
H(96A)	3209(3)	10236(3)	-1036(3)	67
H(90A)	3260(21)	11007(5)	-2121(18)	112
H(90B)	3534(14)	11911(19)	-1744(9)	112
H(90C)	2681(7)	11790(22)	-2475(10)	112
H(10A)	-1070(4)	8389(4)	-1884(4)	108
H(10C)	-1870(4)	8186(6)	-1215(5)	121
H(10D)	-1718(7)	7015(8)	-482(7)	216
H(10E)	-966(9)	5808(9)	-468(6)	383
H(10F)	-194(4)	6053(4)	-1081(3)	89
H(10G)	-81(40)	7926(9)	-2070(40)	246
H(10H)	-300(30)	7028(40)	-2477(21)	246
H(10I)	495(13)	7148(45)	-1679(22)	246