ORGANOMETALLICS
Organometallics, 1996, 15(10), 2571-2574, DOI:10.1021/om9508703

^{13}C NMR spectral data (δ(ppm))

Compound (solvent)	AlR2	NR'2	(R"N)C(R)(NR")	(R"N)C(R)(NR")	(R"N)C(R)(NR")
1 a	-4.78(br), CH_3	25.98, $CH(\underline{C}H_3)_2$	27.68, $\underline{C}H(CH_3)_2$;	11.57, R = CH_3	174.63
d^8-toluene		48.39, $\underline{C}H(CH_3)_2$	46.87, $\underline{C}H(CH_3)_2$		
1 b	-4.18(br), CH_3	28.40, $CH(\underline{C}H_3)_2$	31.51, $C(\underline{C}H_3)_3$;	19.43, R = CH_3	175.89
d^6-benzene		49.24, $\underline{C}H(CH_3)_2$	33.10, $\underline{C}(CH_3)_3$		
1 c	-3.82(br), CH_3	26.32, $CH(\underline{C}H_3)_2$	125.4, 129.8, 132.3, 146.0,	15.04, R = CH_3	174.09
d^6-benzene		47.54, $\underline{C}H(CH_3)_2$	aryl-C of tolyl		
			20.86, CH_3 of tolyl;		
2 a	-9.77(br), CH_3	13.66, $CH_2\underline{C}H_3$	27.68, $\underline{C}H(CH_3)_2$;	11.20, R = CH_3	174.12
d^8-toluene		40.07, $\underline{C}H_2CH_3$	46.87, $\underline{C}H(CH_3)_2$		
2 b	-10.02(br), CH_3	13.29, $CH_2\underline{C}H_3$	31.52, $C(\underline{C}H_3)_3$;	18.34, R = CH_3	175.44
d^8-toluene		39.90, $\underline{C}H_2CH_3$	32.94, $\underline{C}(CH_3)_3$		
3 a	4.00, $\underline{C}H_2CH_3$	26.18, $CH(\underline{C}H_3)_2$	27.88, $\underline{C}H(CH_3)_2$;	12.47, $CH_2\underline{C}H_3$;	178.63
d^6-benzene	10.86, $CH_2\underline{C}H_3$	48.38, $\underline{C}H(CH_3)_2$	46.36, $\underline{C}H(CH_3)_2$	18.61, $\underline{C}H_2CH_3$	

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3 b	···, $\underline{C}H_2CH_3$	29.18, 27.96,	31.97, $C(\underline{C}H_3)_3$;	15.47, $CH_2\underline{C}H_3$;	181.96
d^6-benzene	10.90, $CH_2\underline{C}H_3$	$\underline{C}H(CH_3)_2$	33.73, $\underline{C}(CH_3)_3$	18.61, $\underline{C}H_2CH_3$	
		49.33, $\underline{C}H(CH_3)_2$			

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Table. Crystal Data and Conditions for Crystallographic Data Collection and Structure Refinement

TITLE,	*** IC3636 ***
Formula ,	Al Mg C22 H51 N4
FW ,	422.96
Diffractometer used,	Nonius
Space Group,	Monoclinic P 21/n
a(angstron),	10.648(4)
b(angstron),	22.149(6)
c(angstron),	12.038(3)
beta(deg.),	92.83(3)
V(A**3),	2835.6(15)
Z ,	4
Dcalc(g.cm-3),	0.991
lambda(Angstron),	0.7107
F(000) ,	944.
Unit cell detn: #;(2theta range),	25;(14.00 - 23.10 deg.)
Scan type,	theta/2theta
Scan width (deg),	2(0.60+0.35tan(theta))
Scan Speed (deg/min),	3.30-8.24
2 Theta(max),	45.0
h k l ranges ,	(-11; 11)(0; 23)(0; 12)
mu(cm-1),	1.025
Crystal size(mm),	0.50 X 0.50 X 0.50
Transmission,	0.975; 1.000
Temperature,	298.00
# of meas. reflns,	3721
# of obsed relfns (I > 2.0sig(I)),	1488
# of unique reflns,	3687
RF;RW ,	0.079;0.079
GoF,	1.38
Refinement program,	NRCVAX
# of atoms,	79
# of refined params,	254 (1488 out of 3687 reflns.)
Minimize function,	SUM(w|Fo-Fc|**2)
Unit weights were used	
g (2nd. ext. coeff.) x 10e4,	1.99(8)
(delta/sigma)max ,	0.0037
(D-map)max.min e/A**3 ,	-0.240; 0.340

NOTE :

RF = Sum(Fo-Fc)/Sum(Fo)

Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]

GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]

3 standard reflns monitored every 1800 seconds, intensity decay 18%.

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Table : Bond Distances and Bond Angles of IC3636

Al-Mg	2.848(4)	N4-C15	1.319(12)
Al-N1	1.945(8)	N4-C20	1.440(12)
Al-N2	1.958(8)	C3-C4	1.529(15)
Al-C1	1.968(12)	C3-C5	1.526(15)
Al-C2	1.971(11)	C6-C7	1.518(18)
Mg-N1	2.155(7)	C6-C8	1.340(22)
Mg-N2	2.152(8)	C9-C10	1.494(16)
Mg-N3	2.062(8)	C9-C11	1.407(20)
Mg-N4	2.079(8)	C12-C13	1.519(17)
Mg-C15	2.439(10)	C12-C14	1.548(17)
N1-C3	1.493(12)	C15-C16	1.536(14)
N1-C6	1.482(14)	C17-C18	1.44(3)
N2-C9	1.471(13)	C17-C19	1.477(22)
N2-C12	1.483(12)	C20-C21	1.446(20)
N3-C15	1.324(12)	C20-C22	1.388(21)
N3-C17	1.461(13)		

Mg-Al-N1	49.12(22)	Mg-N2-C9	113.1(6)
Mg-Al-N2	49.02(22)	Mg-N2-C12	106.3(6)
Mg-Al-C1	109.7(4)	C9-N2-C12	116.7(8)
Mg-Al-C2	140.1(4)	Mg-N3-C15	89.4(6)
N1-Al-N2	96.6(3)	Mg-N3-C17	148.7(7)
N1-Al-C1	108.4(4)	C15-N3-C17	121.8(8)
N1-Al-C2	116.4(5)	Mg-N4-C15	88.8(5)
N2-Al-C1	110.3(5)	Mg-N4-C20	149.5(6)
N2-Al-C2	114.2(4)	C15-N4-C20	121.6(8)
C1-Al-C2	110.2(6)	N1-C3-C4	114.5(9)
Al-Mg-N1	43.03(20)	N1-C3-C5	115.6(9)
Al-Mg-N2	43.39(20)	C4-C3-C5	108.5(9)
Al-Mg-N3	165.1(3)	N1-C6-C7	117.6(10)
Al-Mg-N4	129.24(24)	N1-C6-C8	118.0(11)
Al-Mg-C15	162.0(3)	C7-C6-C8	114.2(12)
N1-Mg-N2	85.1(3)	N2-C9-C10	119.0(10)
N1-Mg-N3	131.4(3)	N2-C9-C11	118.6(10)
N1-Mg-N4	122.9(3)	C10-C9-C11	111.4(11)
N1-Mg-C15	136.5(3)	N2-C12-C13	114.1(9)
N2-Mg-N3	134.0(3)	N2-C12-C14	115.5(9)
N2-Mg-N4	122.9(3)	C13-C12-C14	109.9(10)
N2-Mg-C15	136.6(3)	Mg-C15-N3	57.7(5)
N3-Mg-N4	65.6(3)	Mg-C15-N4	58.5(5)
N3-Mg-C15	32.9(3)	Mg-C15-C16	178.9(8)
N4-Mg-C15	32.7(3)	N3-C15-N4	116.2(8)
Al-N1-Mg	87.9(3)	N3-C15-C16	121.6(9)
Al-N1-C3	115.9(6)	N4-C15-C16	122.2(9)
Al-N1-C6	118.6(7)	N3-C17-C18	109.7(13)
Mg-N1-C3	105.6(5)	N3-C17-C19	110.7(10)
Mg-N1-C6	112.2(6)	C18-C17-C19	108.2(15)
C3-N1-C6	113.0(8)	N4-C20-C21	111.1(10)
Al-N2-Mg	87.6(3)	N4-C20-C22	111.5(11)
Al-N2-C9	114.3(6)	C21-C20-C22	106.0(16)
Al-N2-C12	114.9(6)		

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Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
Al	0.2489(3)	0.81066(14)	0.11799(24)	5.58(14)
Mg	0.2363(3)	0.89330(13)	0.29837(24)	4.79(14)
N1	0.1168(7)	0.8253 (3)	0.2206 (6)	5.4 (4)
N2	0.3813(6)	0.8551 (3)	0.2017 (6)	5.1 (4)
N3	0.2349(8)	0.9331 (3)	0.4531 (6)	7.1 (5)
N4	0.1918(7)	0.9847 (3)	0.2955 (6)	6.0 (4)
C1	0.2036(11)	0.8522 (6)	-0.0229 (9)	9.8 (8)
C2	0.2901(12)	0.7255 (5)	0.0896 (11)	9.8 (8)
C3	0.0038(9)	0.8583 (5)	0.1739 (9)	6.9 (6)
C4	-0.0786(10)	0.8858 (6)	0.2612 (11)	10.1 (8)
C5	-0.0802(12)	0.8230 (6)	0.0907 (11)	10.5 (8)
C6	0.0852(12)	0.7768 (6)	0.2992 (10)	9.5 (7)
C7	0.0128(15)	0.7227 (6)	0.2525 (13)	13.7 (11)
C8	0.1695(21)	0.7634 (8)	0.3818 (13)	19.3 (15)
C9	0.4697(10)	0.8167 (5)	0.2677 (9)	8.5 (7)
C10	0.5776(11)	0.7885 (6)	0.2121 (12)	11.5 (9)
C11	0.5039(17)	0.8340 (9)	0.3775 (14)	18.6 (15)
C12	0.4364(9)	0.9061 (5)	0.1407 (9)	7.4 (6)
C13	0.5126(11)	0.9497 (6)	0.2143 (13)	11.0 (9)
C14	0.5119(13)	0.8883 (7)	0.0391 (12)	12.7 (10)
C15	0.2070(10)	0.9855 (4)	0.4049 (8)	6.7 (6)
C16	0.1910(14)	1.0433 (5)	0.4731 (10)	10.8 (9)
C17	0.2476(16)	0.9269 (5)	0.5740 (9)	12.1 (10)
C18	0.3788(22)	0.9256 (10)	0.6095 (13)	22.2 (18)
C19	0.1891(23)	0.8702 (9)	0.6101 (10)	20.6 (18)
C20	0.1574(12)	1.0383 (5)	0.2333 (8)	8.6 (7)
C21	0.0709(23)	1.0242 (8)	0.1405 (19)	25.1 (18)
C22	0.2613(18)	1.0647 (9)	0.1878 (19)	21.7 (17)
H1a	0.184	0.893	-0.008	10.5
H1b	0.273	0.850	-0.070	10.5
H1c	0.133	0.833	-0.058	10.5
H2a	0.312	0.706	0.158	10.4
H2b	0.219	0.706	0.054	10.4
H2c	0.359	0.724	0.043	10.4
H3	0.035	0.891	0.133	7.7
H4a	-0.027	0.908	0.313	10.9
H4b	-0.138	0.912	0.225	10.9
H4c	-0.120	0.855	0.298	10.9
H5a	-0.030	0.806	0.037	10.9
H5b	-0.122	0.792	0.129	10.9
H5c	-0.140	0.850	0.056	10.9
H6	0.020	0.797	0.336	10.2
H7a	-0.043	0.735	0.194	14.3
H7b	0.069	0.693	0.229	14.3
H7c	-0.035	0.706	0.311	14.3
H8a	0.206	0.800	0.406	19.5
H8b	0.119	0.748	0.441	19.5
H8c	0.223	0.736	0.359	19.5
H9	0.418	0.783	0.278	9.1
H10a	0.551	0.778	0.138	12.1
H10b	0.645	0.815	0.212	12.1
H10c	0.601	0.753	0.252	12.1
H11a	0.432	0.851	0.409	20.3
H11b	0.526	0.798	0.418	20.3
H11c	0.570	0.861	0.378	20.3
H12	0.367	0.929	0.111	8.2

H13a	0.467	0.960	0.276	11.6
H13b	0.590	0.931	0.238	11.6
H13c	0.531	0.985	0.172	11.6
H14a	0.463	0.861	-0.007	13.4
H14b	0.528	0.924	-0.003	13.4
H14c	0.588	0.870	0.063	13.4
H16a	0.110	1.059	0.458	11.4
H16b	0.202	1.034	0.550	11.4
H16c	0.253	1.072	0.454	11.4
H17	0.205	0.960	0.607	12.4
H18a	0.415	0.963	0.587	22.8
H18b	0.384	0.924	0.688	22.8
H18c	0.417	0.893	0.577	22.8
H19a	0.106	0.870	0.588	21.3
H19b	0.235	0.838	0.578	21.3
H19c	0.202	0.868	0.689	21.3
H20	0.121	1.066	0.283	9.0
H21a	-0.002	1.007	0.171	27.1
H21b	0.048	1.063	0.108	27.1
H21c	0.108	1.000	0.093	27.1
H22a	0.321	1.074	0.245	22.5
H22b	0.293	1.037	0.136	22.5
H22c	0.233	1.101	0.151	22.5

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Al	7.43(20)	7.30(20)	6.47(18)	0.74(19)	0.18(15)	-1.82(17)
Mg	7.28(20)	5.41(18)	5.50(17)	0.19(18)	0.21(16)	-0.41(17)
N1	7.4 (5)	6.2 (5)	7.0 (5)	-1.3 (4)	0.4 (4)	-0.5 (4)
N2	6.6 (5)	6.0 (5)	6.9 (5)	0.8 (4)	-0.2 (4)	0.1 (4)
N3	14.6 (8)	6.4 (5)	5.7 (5)	1.9 (6)	-0.8 (5)	-0.8 (4)
N4	10.2 (7)	5.4 (5)	7.0 (5)	1.3 (5)	-0.2 (5)	0.4 (4)
C1	12.0 (10)	18.4 (13)	6.6 (7)	0.5 (10)	-0.4 (7)	0.2 (8)
C2	12.7 (11)	9.0 (9)	15.4 (12)	0.6 (8)	-1.0 (9)	-5.3 (8)
C3	5.8 (7)	9.5 (8)	11.1 (8)	-0.3 (6)	-0.1 (6)	-1.2 (7)
C4	6.5 (7)	14.9 (12)	17.3 (13)	1.9 (8)	4.1 (8)	-2.5 (10)
C5	11.2 (10)	12.8 (11)	15.2 (12)	-0.7 (9)	-4.3 (9)	-2.0 (10)
C6	13.9 (11)	12.1 (11)	10.0 (9)	-2.8 (9)	-2.2 (8)	0.9 (8)
C7	20.1 (16)	13.0 (13)	18.3 (15)	-7.9 (12)	-3.8 (12)	3.0 (11)
C8	39.6 (28)	17.9 (16)	15.2 (14)	-17.6 (19)	-5.4 (16)	7.1 (13)
C9	9.1 (8)	13.0 (10)	9.8 (9)	3.9 (8)	-2.3 (7)	-3.1 (8)
C10	9.6 (10)	16.5 (14)	17.5 (13)	5.3 (10)	-0.9 (9)	-2.1 (11)
C11	22.7 (19)	29.9 (25)	17.4 (17)	16.9 (19)	-4.3 (14)	-0.9 (16)
C12	8.2 (8)	8.2 (8)	11.7 (9)	-1.0 (7)	1.2 (7)	0.7 (7)
C13	8.9 (9)	11.1 (11)	21.7 (15)	-3.4 (8)	1.1 (10)	0.7 (10)
C14	14.0 (12)	19.5 (15)	15.3 (13)	0.5 (12)	8.3 (11)	4.1 (12)
C15	10.8 (9)	6.7 (7)	8.0 (7)	1.5 (6)	0.7 (7)	-0.8 (6)
C16	24.1 (17)	6.6 (8)	10.4 (10)	3.3 (9)	0.5 (10)	-2.9 (7)
C17	31.0 (19)	8.2 (9)	6.3 (8)	-0.7 (11)	-5.3 (10)	-0.2 (7)
C18	38.6 (30)	31.4 (27)	12.7 (14)	-10.2 (23)	-15.1 (17)	1.1 (15)
C19	48.1 (34)	25.0 (21)	5.0 (9)	-8.7 (22)	0.5 (14)	3.6 (11)
C20	18.1 (13)	7.4 (8)	7.2 (8)	-0.4 (8)	0.0 (8)	1.7 (6)
C21	41.8 (32)	14.1 (15)	36.5 (28)	-4.6 (18)	-28.9 (26)	13.8 (17)
C22	21.3 (19)	23.0 (20)	39.0 (30)	9.0 (16)	9.5 (19)	24.3 (22)
H1a	13.3					
H1b	13.3					
H1c	13.3					
H2a	13.2					
H2b	13.2					
H2c	13.2					
H3	9.7					
H4a	13.8					
H4b	13.8					
H4c	13.8					
H5a	13.8					
H5b	13.8					
H5c	13.8					
H6	12.9					
H7a	18.2					
H7b	18.2					
H7c	18.2					
H8a	24.7					
H8b	24.7					
H8c	24.7					
H9	11.6					
H10a	15.4					
H10b	15.4					
H10c	15.4					
H11a	25.7					
H11b	25.7					
H11c	25.7					

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H12	10.3
H13a	14.7
H13b	14.7
H13c	14.7
H14a	17.0
H14b	17.0
H14c	17.0
H16a	14.4
H16b	14.4
H16c	14.4
H17	15.7
H18a	28.8
H18b	28.8
H18c	28.8
H19a	26.9
H19b	26.9
H19c	26.9
H20	11.4
H21a	34.3
H21b	34.3
H21c	34.3
H22a	28.5
H22b	28.5
H22c	28.5

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

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S

Table. Crystal Data and Conditions for Crystallographic Data Collection and Structure Refinement

TITLE,	*** IC3523 ***
Formula ,	Al Mg C24 H55 N4
FW ,	451.01
Diffractometer used,	Nonius
Space Group,	Monoclinic P 21/n
a(angstron),	9.912(5)
b(angstron),	19.648(4)
c(angstron),	15.296(4)
beta(deg.),	92.19(3)
V(A**3),	2976.8(18)
Z ,	4
Dcalc(g.cm-3),	1.006
lambda(Angstron),	0.7107
F(000) ,	1009.
Unit cell detn: #;(2theta range),	25;(17.10 - 24.68 deg.)
Scan type,	theta/2theta
Scan width (deg),	2(0.60+0.35tan(theta))
Scan Speed (deg/min),	3.30-8.24
2 Theta(max),	45.0
h k l ranges ,	(-10; 10)(0; 21)(0; 16)
mu(cm-1),	1.009
Crystal size(mm),	0.30 X 0.50 X 0.50
Transmission,	0.803; 1.000
Temperature,	298.00
# of meas. reflns,	3881
# of obsed relfns (I > 2.0sig(I)),	1808
# of unique reflns,	3881
RF;RW ,	0.060;0.058
GoF,	1.40
Refinement program,	NRCVAX
# of atoms,	89
# of refined params,	280 (1808 out of 3881 reflns.)
Minimize function,	SUM(w|Fo-Fc|**2)
Unit weights were used	
(delta/sigma)max ,	0.0097
(D-map)max.min e/A**3 ,	-0.180; 0.370

NOTE :

RF = Sum(Fo-Fc)/Sum(Fo)

Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)]

GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]

3 standard reflns monitored every 3600 seconds, intensity decay 30%.

☆ Disorder for C8(2/3) and C8'(1/3).

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IC3523

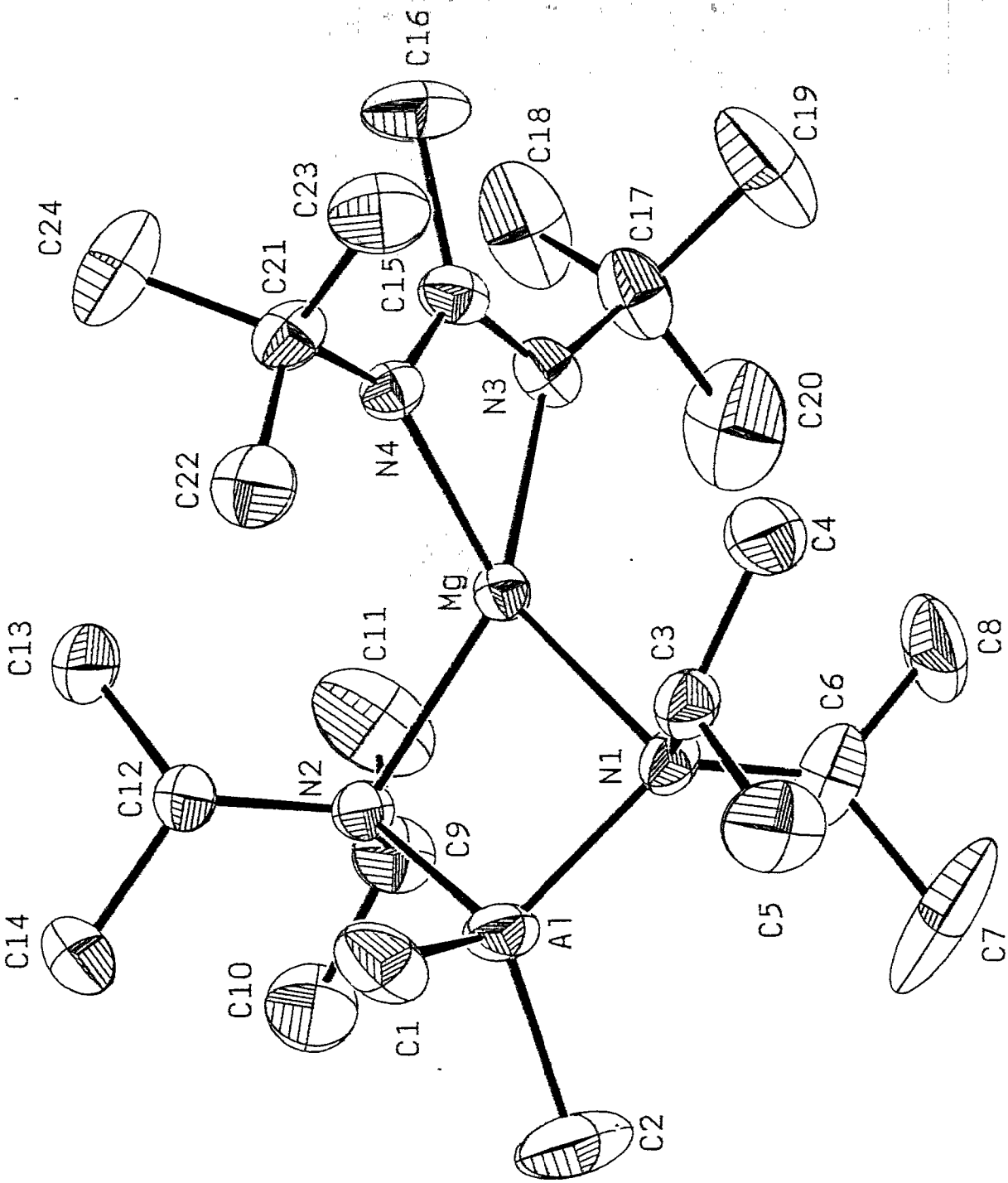

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Table : Bond Distances and Bond Angles of IC3523

Al-Mg	2.865(3)	N4-C21	1.472(8)
Al-N1	1.950(6)	C3-C4	1.512(10)
Al-N2	1.974(5)	C3-C5	1.545(10)
Al-C1	1.979(10)	C6-C7	1.530(13)
Al-C2	1.953(9)	C6-C8	1.345(16)
Mg-N1	2.174(5)	C6-C8'	1.52(3)
Mg-N2	2.160(5)	C9-C10	1.513(11)
Mg-N3	2.064(5)	C9-C11	1.447(13)
Mg-N4	2.063(5)	C12-C13	1.517(10)
Mg-C15	2.446(6)	C12-C14	1.527(10)
N1-C3	1.486(8)	C15-C16	1.532(10)
N1-C6	1.481(9)	C17-C18	1.511(11)
N2-C9	1.481(9)	C17-C19	1.521(12)
N2-C12	1.494(8)	C17-C20	1.492(15)
N3-C15	1.328(9)	C21-C22	1.501(11)
N3-C17	1.463(8)	C21-C23	1.513(10)
N4-C15	1.323(8)	C21-C24	1.539(10)

Mg-Al-N1	49.32(15)	Mg-N3-C17	144.8(5)
Mg-Al-N2	48.88(15)	C15-N3-C17	125.5(6)
Mg-Al-C1	110.0(3)	Mg-N4-C15	89.8(4)
Mg-Al-C2	139.8(4)	Mg-N4-C21	144.1(4)
N1-Al-N2	96.50(21)	C15-N4-C21	126.1(5)
N1-Al-C1	108.7(3)	N1-C3-C4	116.7(6)
N1-Al-C2	117.2(4)	N1-C3-C5	115.3(6)
N2-Al-C1	110.8(3)	C4-C3-C5	108.7(6)
N2-Al-C2	112.7(3)	N1-C6-C7	115.0(8)
C1-Al-C2	110.2(5)	N1-C6-C8	122.3(9)
Al-Mg-N1	42.87(15)	N1-C6-C8'	120.9(10)
Al-Mg-N2	43.52(13)	C7-C6-C8	104.3(10)
Al-Mg-N3	163.10(19)	C7-C6-C8'	105.4(12)
Al-Mg-N4	131.27(17)	C8-C6-C8'	83.9(13)
Al-Mg-C15	164.01(19)	N2-C9-C10	119.0(7)
N1-Mg-N2	85.00(19)	N2-C9-C11	115.8(7)
N1-Mg-N3	130.87(22)	C10-C9-C11	108.3(7)
N1-Mg-N4	126.02(20)	N2-C12-C13	113.4(6)
N1-Mg-C15	138.16(21)	N2-C12-C14	117.2(6)
N2-Mg-N3	132.64(20)	C13-C12-C14	109.0(6)
N2-Mg-N4	122.55(21)	Mg-C15-N3	57.5(3)
N2-Mg-C15	135.79(20)	Mg-C15-N4	57.5(3)
N3-Mg-N4	65.62(21)	Mg-C15-C16	176.9(5)
N3-Mg-C15	32.88(22)	N3-C15-N4	115.0(5)
N4-Mg-C15	32.75(21)	N3-C15-C16	122.3(6)
Al-N1-Mg	87.81(19)	N4-C15-C16	122.7(6)
Al-N1-C3	113.7(4)	N3-C17-C18	114.8(6)
Al-N1-C6	118.4(5)	N3-C17-C19	113.6(6)
Mg-N1-C3	106.5(4)	N3-C17-C20	106.9(7)
Mg-N1-C6	111.2(4)	C18-C17-C19	111.1(7)
C3-N1-C6	115.2(5)	C18-C17-C20	105.1(8)
Al-N2-Mg	87.60(19)	C19-C17-C20	104.4(8)
Al-N2-C9	114.2(4)	N4-C21-C22	106.4(5)
Al-N2-C12	111.1(4)	N4-C21-C23	113.3(6)
Mg-N2-C9	110.9(4)	N4-C21-C24	113.0(6)
Mg-N2-C12	110.2(4)	C22-C21-C23	106.9(6)
C9-N2-C12	118.6(5)	C22-C21-C24	106.5(7)
Mg-N3-C15	89.6(4)	C23-C21-C24	110.2(7)

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Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
Al	0.78670(24)	0.97935(11)	0.18181(15)	6.68(11)
Mg	0.66848(20)	1.08667(10)	0.27992(13)	4.48(9)
N1	0.7748 (5)	1.0768 (3)	0.1589 (3)	5.27(25)
N2	0.6530 (5)	0.97709(24)	0.2742 (3)	5.02(24)
N3	0.5396 (5)	1.16132(25)	0.3219 (3)	5.6 (3)
N4	0.7371 (5)	1.13765(24)	0.3908 (3)	4.73(23)
C1	0.9697 (9)	0.9584 (4)	0.2308 (6)	10.1 (5)
C2	0.7404 (12)	0.9181 (5)	0.0847 (6)	13.7 (7)
C3	0.9052 (7)	1.1133 (4)	0.1727 (4)	6.3 (4)
C4	0.8976 (9)	1.1890 (4)	0.1897 (5)	9.0 (5)
C5	1.0102 (9)	1.1004 (5)	0.1025 (6)	11.0 (6)
C6	0.6901 (8)	1.1003 (5)	0.0829 (5)	9.7 (6)
C7	0.7449 (13)	1.0831 (10)	-0.0066 (6)	22.0 (15)
C8	0.6473 (14)	1.1650 (7)	0.0747 (9)	11.3 (9)
C8'	0.5403 (24)	1.0836 (14)	0.0756 (15)	9.4 (16)
C9	0.5160 (7)	0.9558 (4)	0.2433 (5)	7.7 (4)
C10	0.4864 (9)	0.8808 (4)	0.2315 (6)	10.4 (6)
C11	0.4053 (10)	0.9865 (5)	0.2880 (8)	14.0 (8)
C12	0.7120 (7)	0.9463 (3)	0.3563 (4)	6.2 (4)
C13	0.6334 (9)	0.9630 (4)	0.4368 (5)	9.1 (5)
C14	0.7414 (8)	0.8700 (4)	0.3552 (5)	8.4 (5)
C15	0.6253 (6)	1.1745 (3)	0.3887 (4)	5.6 (3)
C16	0.5941 (9)	1.2266 (4)	0.4596 (6)	10.1 (5)
C17	0.4124 (7)	1.1971 (4)	0.3028 (5)	8.1 (5)
C18	0.3044 (8)	1.1849 (6)	0.3681 (8)	13.5 (7)
C19	0.4301 (10)	1.2726 (5)	0.2851 (9)	14.6 (8)
C20	0.3557 (9)	1.1691 (7)	0.2184 (7)	14.6 (8)
C21	0.8506 (6)	1.1439 (4)	0.4552 (4)	6.1 (4)
C22	0.9554 (7)	1.0936 (4)	0.4286 (5)	8.3 (5)
C23	0.9166 (8)	1.2133 (4)	0.4556 (6)	9.7 (5)
C24	0.8123 (10)	1.1242 (6)	0.5485 (5)	12.3 (7)
H1a	0.995	0.989	0.281	9.6
H1b	0.978	0.913	0.254	9.6
H1c	1.040	0.964	0.190	9.6
H2a	0.649	0.928	0.058	13.1
H2b	0.799	0.922	0.036	13.1
H2c	0.737	0.871	0.100	13.1
H3	0.948	1.094	0.226	7.6
H4a	0.839	1.200	0.236	10.2
H4b	0.988	1.207	0.209	10.2
H4c	0.872	1.214	0.139	10.2
H5a	1.016	1.053	0.089	11.5
H5b	0.980	1.123	0.049	11.5
H5c	1.097	1.117	0.119	11.5
H6	0.611	1.069	0.083	10.6
H7a	0.778	1.034	-0.008	19.7
H7b	0.685	1.087	-0.055	19.7
H7c	0.822	1.110	-0.013	19.7
H8a	0.595	1.175	0.123	11.5
H8b	0.723	1.190	0.064	11.5
H8c	0.586	1.164	0.027	11.5
H8'a	0.493	1.094	0.130	9.2
H8'b	0.501	1.116	0.031	9.2
H8'c	0.513	1.039	0.059	9.2
H9	0.501	0.975	0.183	8.8
H10a	0.558	0.859	0.198	10.8

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H10b	0.487	0.858	0.287	10.8
H10c	0.403	0.870	0.201	10.8
H11a	0.415	1.035	0.298	12.9
H11b	0.316	0.979	0.262	12.9
H11c	0.400	0.967	0.348	12.9
H12	0.801	0.967	0.369	11.0
H13a	0.614	1.012	0.441	10.1
H13b	0.544	0.941	0.434	10.1
H13c	0.676	0.950	0.492	10.1
H14a	0.791	0.856	0.307	9.2
H14b	0.786	0.853	0.408	9.2
H14c	0.655	0.844	0.350	9.2
H16a	0.666	1.230	0.504	10.5
H16b	0.581	1.272	0.436	10.5
H16c	0.513	1.216	0.490	10.5
H18a	0.221	1.208	0.356	13.8
H18b	0.284	1.138	0.376	13.8
H18c	0.336	1.201	0.427	13.8
H19a	0.345	1.295	0.272	14.5
H19b	0.468	1.294	0.337	14.5
H19c	0.488	1.281	0.239	14.5
H20a	0.275	1.187	0.195	13.5
H20b	0.422	1.173	0.169	13.5
H20c	0.344	1.118	0.220	13.5
H22a	1.036	1.093	0.468	9.0
H22b	0.922	1.047	0.430	9.0
H22c	0.987	1.101	0.371	9.0
H23a	0.994	1.217	0.497	10.0
H23b	0.953	1.225	0.399	10.0
H23c	0.855	1.249	0.470	10.0
H24a	0.889	1.127	0.590	12.7
H24b	0.742	1.152	0.569	12.7
H24c	0.782	1.077	0.550	12.7

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

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Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
Al	10.66(18)	6.84(14)	8.14(15)	-0.97(14)	4.02(13)	-1.44(13)
Mg	6.20(12)	5.18(12)	5.68(12)	0.01(11)	0.68(10)	0.33(11)
N1	7.2 (4)	7.6 (4)	5.3 (3)	-1.1 (3)	1.2 (3)	0.3 (3)
N2	7.4 (3)	5.5 (3)	6.3 (3)	-1.3 (3)	1.8 (3)	0.0 (3)
N3	5.1 (3)	6.5 (4)	9.9 (4)	0.7 (3)	2.1 (3)	1.4 (3)
N4	5.7 (3)	6.5 (3)	5.8 (3)	-0.3 (3)	0.9 (3)	-0.5 (3)
C1	12.1 (7)	9.2 (6)	17.6 (9)	2.4 (5)	7.4 (7)	1.4 (6)
C2	24.0 (12)	13.9 (9)	14.7 (9)	-7.2 (9)	10.7 (9)	-7.7 (7)
C3	9.3 (5)	8.2 (5)	6.7 (5)	-1.1 (4)	1.3 (4)	0.5 (4)
C4	15.3 (8)	7.9 (6)	11.3 (7)	-3.0 (5)	3.4 (6)	0.3 (5)
C5	11.5 (7)	14.4 (8)	16.2 (9)	-2.6 (6)	6.9 (6)	-0.3 (7)
C6	11.0 (7)	18.6 (9)	7.3 (5)	-0.9 (7)	0.4 (5)	2.9 (6)
C7	22.4 (14)	56.1 (29)	5.0 (6)	3.9 (17)	0.2 (7)	2.4 (11)
C8	14.3 (12)	14.3 (13)	14.4 (12)	6.1 (10)	0.1 (10)	7.4 (10)
C8'	11.6 (21)	16.0 (25)	8.1 (17)	-2.4 (19)	-2.4 (15)	2.5 (18)
C9	8.7 (6)	9.0 (6)	11.7 (6)	-2.1 (5)	2.5 (5)	-0.1 (5)
C10	15.5 (9)	10.5 (7)	13.1 (8)	-5.3 (6)	-2.0 (6)	-1.0 (6)
C11	10.7 (8)	12.5 (9)	30.0 (15)	-3.0 (7)	1.5 (9)	0.7 (9)
C12	9.9 (6)	7.0 (5)	6.7 (5)	0.1 (4)	1.7 (4)	0.7 (4)
C13	17.5 (9)	9.6 (6)	7.9 (6)	-1.3 (6)	3.6 (6)	1.8 (5)
C14	13.0 (7)	7.0 (5)	11.9 (7)	0.5 (5)	0.6 (6)	1.9 (5)
C15	7.5 (5)	5.4 (4)	8.7 (5)	-0.4 (4)	2.9 (4)	-0.2 (4)
C16	12.6 (7)	11.2 (7)	14.9 (8)	1.1 (6)	4.5 (6)	-5.9 (6)
C17	6.6 (5)	10.1 (6)	14.2 (8)	2.0 (5)	2.2 (5)	4.2 (6)
C18	8.0 (6)	19.0 (11)	24.7 (12)	4.1 (7)	7.7 (7)	10.1 (9)
C19	13.5 (9)	11.1 (8)	31.5 (16)	4.4 (7)	7.3 (9)	9.9 (9)
C20	8.5 (7)	27.4 (15)	19.2 (11)	5.2 (8)	-2.8 (7)	5.1 (11)
C21	7.3 (5)	9.3 (5)	6.6 (5)	-2.7 (4)	0.1 (4)	-1.0 (4)
C22	8.8 (6)	12.0 (7)	10.7 (6)	0.5 (5)	-2.8 (5)	-0.7 (6)
C23	10.7 (7)	11.8 (7)	14.4 (8)	-3.3 (6)	-0.8 (6)	-3.5 (6)
C24	14.6 (9)	25.1 (13)	7.1 (6)	-5.1 (9)	-0.1 (6)	1.3 (7)
H1a	12.2					
H1b	12.2					
H1c	12.2					
H2a	16.6					
H2b	16.6					
H2c	16.6					
H3	9.6					
H4a	12.9					
H4b	12.9					
H4c	12.9					
H5a	14.5					
H5b	14.5					
H5c	14.5					
H6	13.4					
H7a	24.9					
H7b	24.9					
H7c	24.9					
H8a	14.6					
H8b	14.6					
H8c	14.6					
H8'a	11.7					
H8'b	11.7					
H8'c	11.7					
H9	11.1					

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H10a	13.7
H10b	13.7
H10c	13.7
H11a	16.4
H11b	16.4
H11c	16.4
H12	13.9
H13a	12.8
H13b	12.8
H13c	12.8
H14a	11.7
H14b	11.7
H14c	11.7
H16a	13.3
H16b	13.3
H16c	13.3
H18a	17.5
H18b	17.5
H18c	17.5
H19a	18.4
H19b	18.4
H19c	18.4
H20a	17.1
H20b	17.1
H20c	17.1
H22a	11.4
H22b	11.4
H22c	11.4
H23a	12.7
H23b	12.7
H23c	12.7
H24a	16.1
H24b	16.1
H24c	16.1

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)