ORGANOMETALLICS
Organometallics, 1997, 16(25), 5522-5527, DOI:10.1021/om970660l

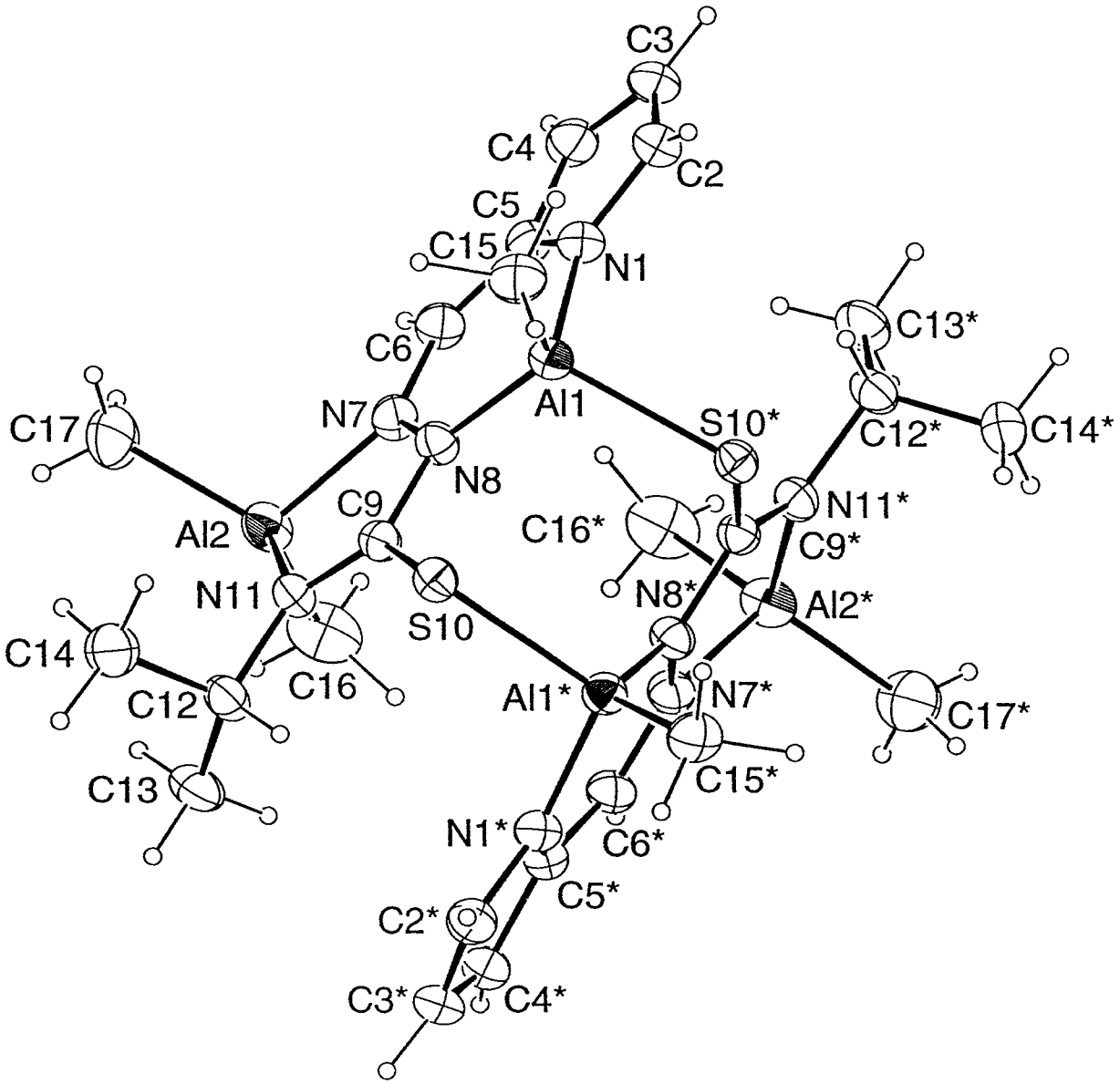


Figure 1. Molecular structure of $\{(MeAl)[NC_4H_3CHNNC(S)N^iC_3H_7](AlMe_3)\}_2$ (**1**). The thermal ellipsoids are drown at the 30% probability level.

Positional parameters for $\{(MeAl)[NC_4H_3CHNNC(S)N^iC_3H_7](AlMe_3)\}_2$

atom	x	y	z
S10	0.52870(5)	-0.08622(4)	0.3596(9)
Al1	0.59131(6)	0.04698(5)	0.4113(9)
Al2	0.61430(7)	-0.09652(6)	0.8113(9)
N1	0.6344(2)	0.1123(2)	0.531(1)
N7	0.6192(2)	-0.0123(2)	0.707(1)
N8	0.5920(2)	-0.0171(2)	0.5627(10)
N11	0.5732(2)	-0.1265(1)	0.631(1)
C2	0.6530(2)	0.1761(2)	0.500(1)
C3	0.6826(2)	0.2083(2)	0.617(1)
C4	0.6838(3)	0.1633(2)	0.729(1)
C5	0.6529(2)	0.1041(2)	0.6769(10)
C6	0.6456(2)	0.0444(2)	0.752(1)
C9	0.5669(2)	-0.0795(2)	0.5347(10)
C12	0.5497(2)	-0.1951(2)	0.597(1)
C13	0.5154(3)	-0.2265(2)	0.731(1)
C14	0.6165(3)	-0.2336(2)	0.541(1)
C15	0.6447(3)	0.0416(3)	0.227(1)
C16	0.5395(4)	-0.0924(3)	0.967(1)
C17	0.7157(3)	-0.1278(3)	0.851(1)
H2	0.648(2)	0.185(2)	0.413(5)
H3	0.695(2)	0.254(2)	0.616(5)
H4	0.700(2)	0.169(2)	0.823(5)
H6	0.661(2)	0.041(2)	0.854(5)
H12	0.513(2)	-0.193(2)	0.514(5)
H13b	0.555(3)	-0.229(2)	0.828(6)
H13c	0.474(3)	-0.201(3)	0.771(6)
H13a	0.499(2)	-0.272(2)	0.703(4)
H14a	0.602(3)	-0.282(3)	0.526(7)
H14b	0.655(3)	-0.233(2)	0.612(5)
H14c	0.638(4)	-0.207(3)	0.440(8)
H15b	0.691(4)	0.004(3)	0.224(8)
H15a	0.668(5)	0.084(4)	0.211(9)
H15c	0.615(5)	0.023(4)	0.145(9)
H16a	0.548(4)	-0.129(4)	1.024(9)
H16b	0.481(6)	-0.088(5)	0.92(1)
H16c	0.548(6)	-0.054(6)	1.02(1)
H17b	0.732(5)	-0.105(4)	0.93(1)
H17a	0.725(3)	-0.168(3)	0.883(7)
H17c	0.754(6)	-0.123(4)	0.758(10)
Al1*	0.40870(6)	-0.04698(5)	0.4113(9)
S10*	0.47130(5)	0.08622(4)	0.3596(9)
N1*	0.3656(2)	-0.1123(2)	0.531(1)
N8*	0.4080(2)	0.0171(2)	0.5627(10)
C15*	0.3553(3)	-0.0416(3)	0.227(1)
C9*	0.4331(2)	0.0795(2)	0.5347(10)
C2*	0.3470(2)	-0.1761(2)	0.500(1)
C5*	0.3471(2)	-0.1041(2)	0.6769(10)
N7*	0.3808(2)	0.0123(2)	0.707(1)
H15b*	0.309(4)	-0.004(3)	0.224(8)
H15a*	0.332(5)	-0.084(4)	0.211(9)
H15c*	0.385(5)	-0.023(4)	0.145(9)
N11*	0.4268(2)	0.1265(1)	0.631(1)
C3*	0.3174(2)	-0.2083(2)	0.617(1)
H2*	0.352(2)	-0.185(2)	0.413(5)
C4*	0.3162(3)	-0.1633(2)	0.729(1)
C6*	0.3544(2)	-0.0444(2)	0.752(1)
Al2*	0.38570(7)	0.09652(6)	0.8113(9)
C12*	0.4503(2)	0.1951(2)	0.597(1)
H3*	0.305(2)	-0.254(2)	0.616(5)

H4*	0.300(2)	-0.169(2)	0.823(5)
H6*	0.339(2)	-0.041(2)	0.854(5)
C16*	0.4605(4)	0.0924(3)	0.967(1)
C17*	0.2843(3)	0.1278(3)	0.851(1)
C13*	0.4846(3)	0.2265(2)	0.731(1)
C14*	0.3835(3)	0.2336(2)	0.541(1)
H12*	0.487(2)	0.193(2)	0.514(5)
H16a*	0.452(4)	0.129(4)	1.024(9)
H16b*	0.519(6)	0.088(5)	0.92(1)
H16c*	0.452(6)	0.054(6)	1.02(1)
H17b*	0.268(5)	0.105(4)	0.93(1)
H17a*	0.275(3)	0.168(3)	0.883(7)
H17c*	0.246(6)	0.123(4)	0.758(10)
H13b*	0.445(3)	0.229(2)	0.828(6)
H13c*	0.526(3)	0.201(3)	0.771(6)
H13a*	0.501(2)	0.272(2)	0.703(4)
H14a*	0.398(3)	0.282(3)	0.526(7)
H14b*	0.345(3)	0.233(2)	0.612(5)
H14c*	0.362(4)	0.207(3)	0.440(8)

Positional parameters and B(eq) for s157rej

atom	x	y	z	B(eq)
S10	0.52870(5)	-0.08622(4)	0.3596(9)	3.19(2)
Al1	0.59131(6)	0.04698(5)	0.4113(9)	3.20(2)
Al2	0.61430(7)	-0.09652(6)	0.8113(9)	4.19(3)
N1	0.6344(2)	0.1123(2)	0.531(1)	3.60(6)
N7	0.6192(2)	-0.0123(2)	0.707(1)	3.45(6)
N8	0.5920(2)	-0.0171(2)	0.5627(10)	3.18(6)
N11	0.5732(2)	-0.1265(1)	0.631(1)	3.34(6)
C2	0.6530(2)	0.1761(2)	0.500(1)	4.32(10)
C3	0.6826(2)	0.2083(2)	0.617(1)	4.73(10)
C4	0.6838(3)	0.1633(2)	0.729(1)	4.48(10)
C5	0.6529(2)	0.1041(2)	0.6769(10)	3.60(7)
C6	0.6456(2)	0.0444(2)	0.752(1)	3.63(8)
C9	0.5669(2)	-0.0795(2)	0.5347(10)	3.01(6)
C12	0.5497(2)	-0.1951(2)	0.597(1)	3.74(8)
C13	0.5154(3)	-0.2265(2)	0.731(1)	4.6(1)
C14	0.6165(3)	-0.2336(2)	0.541(1)	5.7(1)
C15	0.6447(3)	0.0416(3)	0.227(1)	4.37(10)
C16	0.5395(4)	-0.0924(3)	0.967(1)	6.3(1)
C17	0.7157(3)	-0.1278(3)	0.851(1)	6.9(1)
H2	0.648(2)	0.185(2)	0.413(5)	3.5(8)
H3	0.695(2)	0.254(2)	0.616(5)	4.1(8)
H4	0.700(2)	0.169(2)	0.823(5)	4.1(8)
H6	0.661(2)	0.041(2)	0.854(5)	4.3(8)
H12	0.513(2)	-0.193(2)	0.514(5)	5.3(9)
H13b	0.555(3)	-0.229(2)	0.828(6)	6.9(9)
H13c	0.474(3)	-0.201(3)	0.771(6)	6.4(9)
H13a	0.499(2)	-0.272(2)	0.703(4)	4.0(8)
H14a	0.602(3)	-0.282(3)	0.526(7)	8.0(10)
H14b	0.655(3)	-0.233(2)	0.612(5)	4.5(9)
H14c	0.638(4)	-0.207(3)	0.440(8)	10.1(9)
H15b	0.691(4)	0.004(3)	0.224(8)	10.2(9)
H15a	0.668(5)	0.084(4)	0.211(9)	11.6(9)
H15c	0.615(5)	0.023(4)	0.145(9)	11.7(8)
H16a	0.548(4)	-0.129(4)	1.024(9)	11.3(8)
H16b	0.481(6)	-0.088(5)	0.92(1)	17.7(6)
H16c	0.548(6)	-0.054(6)	1.02(1)	17.3(6)
H17b	0.732(5)	-0.105(4)	0.93(1)	13.1(7)
H17a	0.725(3)	-0.168(3)	0.883(7)	8.2(9)
H17c	0.754(6)	-0.123(4)	0.758(10)	12.9(7)
Al1*	0.40870(6)	-0.04698(5)	0.4113(9)	3.20(2)
S10*	0.47130(5)	0.08622(4)	0.3596(9)	3.19(2)
N1*	0.3656(2)	-0.1123(2)	0.531(1)	3.60(6)
N8*	0.4080(2)	0.0171(2)	0.5627(10)	3.18(6)
C15*	0.3553(3)	-0.0416(3)	0.227(1)	4.37(10)
C9*	0.4331(2)	0.0795(2)	0.5347(10)	3.01(6)
C2*	0.3470(2)	-0.1761(2)	0.500(1)	4.32(10)
C5*	0.3471(2)	-0.1041(2)	0.6769(10)	3.60(7)
N7*	0.3808(2)	0.0123(2)	0.707(1)	3.45(6)
H15b*	0.309(4)	-0.004(3)	0.224(8)	10.2(9)
H15a*	0.332(5)	-0.084(4)	0.211(9)	11.6(9)
H15c*	0.385(5)	-0.023(4)	0.145(9)	11.7(8)
N11*	0.4268(2)	0.1265(1)	0.631(1)	3.34(6)
C3*	0.3174(2)	-0.2083(2)	0.617(1)	4.73(10)
H2*	0.352(2)	-0.185(2)	0.413(5)	3.5(8)
C4*	0.3162(3)	-0.1633(2)	0.729(1)	4.48(10)
C6*	0.3544(2)	-0.0444(2)	0.752(1)	3.63(8)
Al2*	0.38570(7)	0.09652(6)	0.8113(9)	4.19(3)
C12*	0.4503(2)	0.1951(2)	0.597(1)	3.74(8)
H3*	0.305(2)	-0.254(2)	0.616(5)	4.1(8)

H4*	0.300(2)	-0.169(2)	0.823(5)	4.1(8)
H6*	0.339(2)	-0.041(2)	0.854(5)	4.3(8)
C16*	0.4605(4)	0.0924(3)	0.967(1)	6.3(1)
C17*	0.2843(3)	0.1278(3)	0.851(1)	6.9(1)
C13*	0.4846(3)	0.2265(2)	0.731(1)	4.6(1)
C14*	0.3835(3)	0.2336(2)	0.541(1)	5.7(1)
H12*	0.487(2)	0.193(2)	0.514(5)	5.3(9)
H16a*	0.452(4)	0.129(4)	1.024(9)	11.3(8)
H16b*	0.519(6)	0.088(5)	0.92(1)	17.7(6)
H16c*	0.452(6)	0.054(6)	1.02(1)	17.3(6)
H17b*	0.268(5)	0.105(4)	0.93(1)	13.1(7)
H17a*	0.275(3)	0.168(3)	0.883(7)	8.2(9)
H17c*	0.246(6)	0.123(4)	0.758(10)	12.9(7)
H13b*	0.445(3)	0.229(2)	0.828(6)	6.9(9)
H13c*	0.526(3)	0.201(3)	0.771(6)	6.4(9)
H13a*	0.501(2)	0.272(2)	0.703(4)	4.0(8)
H14a*	0.398(3)	0.282(3)	0.526(7)	8.0(10)
H14b*	0.345(3)	0.233(2)	0.612(5)	4.5(9)
H14c*	0.362(4)	0.207(3)	0.440(8)	10.1(9)

Intramolecular Distances

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
S10	AL1	2.326(2)	65502	C4	H4	0.92(6)	1
S10	C9	1.755(5)	1	C5	C6	1.398(7)	1
AL1	N1	1.885(4)	1	C6	H6	0.97(6)	1
AL1	N8	1.902(4)	1	C12	C13	1.509(8)	1
AL1	C15	1.944(6)	1	C12	C14	1.512(8)	1
AL2	N7	1.955(4)	1	C12	H12	1.01(6)	1
AL2	N11	1.910(4)	1	C13	H13b	1.14(7)	1
AL2	C16	1.957(7)	1	C13	H13c	0.96(6)	1
AL2	C17	1.946(7)	1	C13	H13a	1.00(5)	1
N1	C2	1.361(6)	1	C14	H14a	1.02(7)	1
N1	C5	1.388(7)	1	C14	H14b	0.95(6)	1
N7	N8	1.416(6)	1	C14	H14c	1.14(9)	1
N7	C6	1.307(6)	1	C15	H15b	1.11(8)	1
N8	C9	1.362(6)	1	C15	H15a	0.96(9)	1
N11	C9	1.305(6)	1	C15	H15c	1.0(1)	1
N11	C12	1.481(6)	1	C16	H16a	0.9(1)	1
C2	C3	1.359(8)	1	C16	H16b	1.1(1)	1
C2	H2	0.83(5)	1	C16	H16c	0.9(1)	1
C3	C4	1.381(9)	1	C17	H17b	0.9(1)	1
C3	H3	0.96(5)	1	C17	H17a	0.87(7)	1
C4	C5	1.402(6)	1	C17	H17c	1.1(1)	1

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles

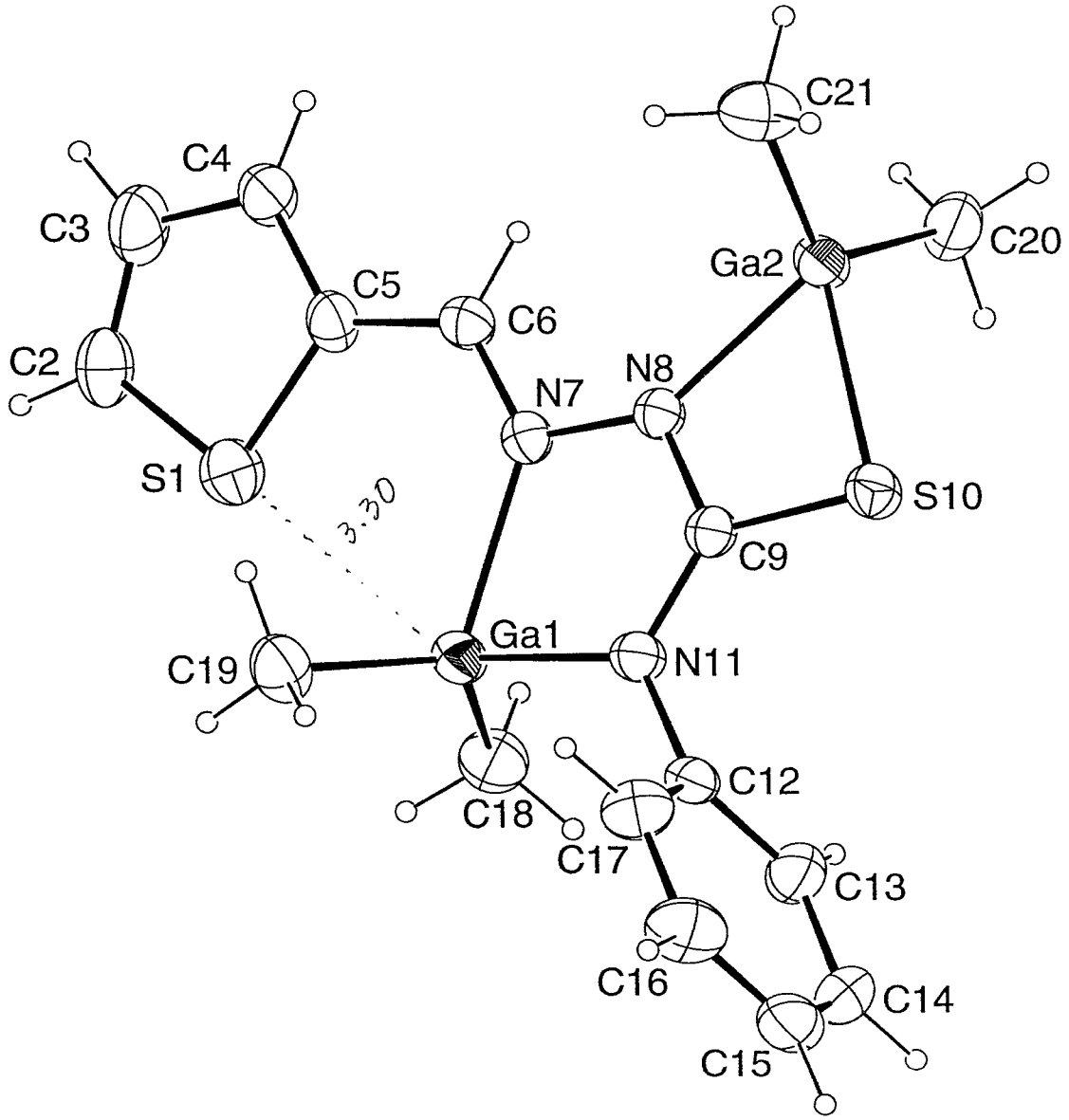
atom	atom	atom	angle	atom	atom	atom	angle
AL1	S10	C9	98.1(2)	N1	C2	H2	113(3)
S10	AL1	N1	104.8(1)	C3	C2	H2	134(3)
S10	AL1	N8	112.8(1)	C2	C3	C4	106.6(5)
S10	AL1	C15	106.8(2)	C2	C3	H3	123(3)
N1	AL1	N8	92.5(2)	C4	C3	H3	130(3)
N1	AL1	C15	110.6(2)	C3	C4	C5	107.2(5)
N8	AL1	C15	126.7(2)	C3	C4	H4	128(3)
N7	AL2	N11	82.3(2)	C5	C4	H4	124(3)
N7	AL2	C16	110.7(3)	N1	C5	C4	108.9(4)
N7	AL2	C17	109.5(3)	N1	C5	C6	124.2(4)
N11	AL2	C16	112.9(3)	C4	C5	C6	126.9(5)
N11	AL2	C17	114.7(3)	N7	C6	C5	129.0(5)
C16	AL2	C17	120.3(4)	N7	C6	H6	110(3)
AL1	N1	C2	129.5(4)	C5	C6	H6	121(3)
AL1	N1	C5	125.3(3)	S10	C9	N8	111.8(3)
C2	N1	C5	105.1(4)	S10	C9	N11	127.1(3)
AL2	N7	N8	112.7(3)	N8	C9	N11	121.1(4)
AL2	N7	C6	128.3(4)	N11	C12	C13	109.6(4)
N8	N7	C6	118.9(4)	N11	C12	C14	109.3(4)
AL1	N8	N7	130.0(3)	N11	C12	H12	107(3)
AL1	N8	C9	119.3(3)	C13	C12	C14	112.5(5)
N7	N8	C9	110.6(3)	C13	C12	H12	112(3)
AL2	N11	C9	113.2(3)	C14	C12	H12	106(3)
AL2	N11	C12	126.0(3)	C12	C13	H13b	114(3)
C9	N11	C12	120.8(4)	C12	C13	H13c	113(4)
N1	C2	C3	112.2(5)	C12	C13	H13a	107(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles cont

atom	atom	atom	angle	atom	atom	atom	angle
H13b	C13	H13c	101(5)	H17a	C17	H17c	103(7)
H13b	C13	H13a	110(4)				
H13c	C13	H13a	111(5)				
C12	C14	H14a	110(4)				
C12	C14	H14b	108(3)				
C12	C14	H14c	108(4)				
H14a	C14	H14b	107(5)				
H14a	C14	H14c	116(6)				
H14b	C14	H14c	108(5)				
AL1	C15	H15b	115(5)				
AL1	C15	H15a	107(6)				
AL1	C15	H15c	115(6)				
H15b	C15	H15a	106(7)				
H15b	C15	H15c	97(7)				
H15a	C15	H15c	116(7)				
AL2	C16	H16a	106(6)				
AL2	C16	H16b	112(7)				
AL2	C16	H16c	108(8)				
H16a	C16	H16b	115(8)				
H16a	C16	H16c	110(10)				
H16b	C16	H16c	106(10)				
AL2	C17	H17b	106(6)				
AL2	C17	H17a	122(4)				
AL2	C17	H17c	114(6)				
H17b	C17	H17a	99(8)				
H17b	C17	H17c	111(8)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.


C21
C4
C3
C20
Ga2
C5
C6
C2
N8
N7
S1
S10
3.30
C9
Ga1
C19
N11
C12
C18
C17
C13
C16
C14
C15

Positional parameters and B(eq) for $(Me_2Ga)[SC_4H_3CHNNC(S)NC_6H_5](GaMe_2)$

atom	x	y	z	B(eq)
Ga1	0.92130(2)	0.07156(2)	0.63067(4)	3.54(1)
Ga2	0.72858(2)	0.24331(2)	0.60596(4)	3.62(1)
S1	0.98986(7)	0.11641(6)	0.9018(1)	5.03(3)
S10	0.73640(5)	0.16828(5)	0.43025(9)	3.68(2)
N7	0.8685(2)	0.1571(1)	0.7035(3)	3.02(6)
N8	0.8122(2)	0.1765(1)	0.6275(2)	3.08(7)
N11	0.8506(2)	0.0892(1)	0.4987(3)	3.36(7)
C2	1.0304(2)	0.1471(3)	1.0312(4)	5.1(1)
C3	1.0031(3)	0.2065(3)	1.0648(5)	6.3(1)
C4	0.9488(2)	0.2304(3)	0.9864(4)	5.5(1)
C5	0.9349(2)	0.1852(2)	0.8916(3)	3.82(9)
C6	0.8802(2)	0.1957(2)	0.7995(3)	3.61(9)
C9	0.8058(2)	0.1392(2)	0.5222(3)	2.96(8)
C12	0.8443(2)	0.0512(2)	0.3855(3)	3.42(8)
C13	0.7984(2)	-0.0033(2)	0.3806(4)	4.7(1)
C14	0.7944(3)	-0.0416(2)	0.2724(5)	6.0(1)
C15	0.8354(3)	-0.0250(3)	0.1711(4)	5.4(1)
C16	0.8814(3)	0.0291(3)	0.1775(4)	5.6(1)
C17	0.8857(3)	0.0667(2)	0.2848(4)	4.6(1)
C18	0.8962(3)	-0.0080(2)	0.7296(5)	5.2(1)
C19	1.0174(2)	0.0967(2)	0.5729(4)	4.9(1)
C20	0.6483(2)	0.2221(2)	0.7156(4)	5.1(1)
C21	0.7575(3)	0.3346(2)	0.5653(4)	5.6(1)
H2	1.0675	0.1249	1.0746	6.1916
H3	1.0195	0.2307	1.1364	7.5557
H4	0.9248	0.2708	0.9992	7.2814
H6	0.8497	0.2339	0.8096	4.3142
H13	0.7697	-0.0144	0.4500	5.7097
H14	0.7627	-0.0795	0.2689	7.0970
H15	0.8319	-0.0508	0.0968	6.4756
H16	0.9101	0.0403	0.1077	6.8359
H17	0.9178	0.1032	0.2888	5.7227
H18a	0.9387	-0.0312	0.7520	6.3844
H18b	0.8666	-0.0370	0.6807	6.3844
H18c	0.8711	0.0058	0.8013	6.3844
H19a	1.0271	0.1420	0.5973	5.9634
H19b	1.0192	0.0933	0.4852	5.9634
H19c	1.0517	0.0674	0.6092	5.9634
H20b	0.6378	0.1752	0.7091	6.4427
H20a	0.6079	0.2477	0.6911	6.4427
H20c	0.6612	0.2327	0.7984	6.4427
H21a	0.7342	0.3657	0.6207	7.0591
H21b	0.8079	0.3392	0.5749	7.0591
H21c	0.7443	0.3450	0.4826	7.0591

Positional parameters for Compound #s131

atom	x	y	z
Ga1	0.92130(2)	0.07156(2)	0.63067(4)
Ga2	0.72858(2)	0.24331(2)	0.60596(4)
S1	0.98986(7)	0.11641(6)	0.9018(1)
S10	0.73640(5)	0.16828(5)	0.43025(9)
N7	0.8685(2)	0.1571(1)	0.7035(3)
N8	0.8122(2)	0.1765(1)	0.6275(2)
N11	0.8506(2)	0.0892(1)	0.4987(3)
C2	1.0304(2)	0.1471(3)	1.0312(4)
C3	1.0031(3)	0.2065(3)	1.0648(5)
C4	0.9488(2)	0.2304(3)	0.9864(4)
C5	0.9349(2)	0.1852(2)	0.8916(3)
C6	0.8802(2)	0.1957(2)	0.7995(3)
C9	0.8058(2)	0.1392(2)	0.5222(3)
C12	0.8443(2)	0.0512(2)	0.3855(3)
C13	0.7984(2)	-0.0033(2)	0.3806(4)
C14	0.7944(3)	-0.0416(2)	0.2724(5)
C15	0.8354(3)	-0.0250(3)	0.1711(4)
C16	0.8814(3)	0.0291(3)	0.1775(4)
C17	0.8857(3)	0.0667(2)	0.2848(4)
C18	0.8962(3)	-0.0080(2)	0.7296(5)
C19	1.0174(2)	0.0967(2)	0.5729(4)
C20	0.6483(2)	0.2221(2)	0.7156(4)
C21	0.7575(3)	0.3346(2)	0.5653(4)
H2	1.0675	0.1249	1.0746
H3	1.0195	0.2307	1.1364
H4	0.9248	0.2708	0.9992
H6	0.8497	0.2339	0.8096
H13	0.7697	-0.0144	0.4500
H14	0.7627	-0.0795	0.2689
H15	0.8319	-0.0508	0.0968
H16	0.9101	0.0403	0.1077
H17	0.9178	0.1032	0.2888
H18a	0.9387	-0.0312	0.7520
H18b	0.8666	-0.0370	0.6807
H18c	0.8711	0.0058	0.8013
H19a	1.0271	0.1420	0.5973
H19b	1.0192	0.0933	0.4852
H19c	1.0517	0.0674	0.6092
H20b	0.6378	0.1752	0.7091
H20a	0.6079	0.2477	0.6911
H20c	0.6612	0.2327	0.7984
H21a	0.7342	0.3657	0.6207
H21b	0.8079	0.3392	0.5749
H21c	0.7443	0.3450	0.4826

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
GA1	N7	2.109(3)	N8	C9	1.358(4)
GA1	N11	1.968(3)	N11	C9	1.317(4)
GA1	C18	1.956(5)	N11	C12	1.436(5)
GA1	C19	1.959(4)	C2	C3	1.331(7)
GA2	S10	2.407(1)	C3	C4	1.399(6)
GA2	N8	2.056(3)	C4	C5	1.380(5)
GA2	C20	1.950(4)	C5	C6	1.436(5)
GA2	C21	1.936(5)	C12	C13	1.376(6)
S1	C2	1.696(5)	C12	C17	1.365(6)
S1	C5	1.707(4)	C13	C14	1.391(6)
S10	C9	1.727(4)	C14	C15	1.371(7)
N7	N8	1.384(4)	C15	C16	1.372(7)
N7	C6	1.302(4)	C16	C17	1.376(6)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bord Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
N7	GA1	N11	79.2(1)	GA1	N11	C12	125.0(2)
N7	GA1	C18	109.4(2)	C9	N11	C12	120.3(3)
N7	GA1	C19	109.9(2)	S1	C2	C3	111.6(3)
N11	GA1	C18	112.1(2)	C2	C3	C4	114.3(4)
N11	GA1	C19	109.7(2)	C3	C4	C5	111.3(4)
C18	GA1	C19	126.5(2)	S1	C5	C4	110.9(3)
S10	GA2	N8	69.27(8)	S1	C5	C6	125.8(3)
S10	GA2	C20	112.8(1)	C4	C5	C6	123.4(4)
S10	GA2	C21	112.4(1)	N7	C6	C5	125.6(3)
N8	GA2	C20	112.0(2)	S10	C9	N8	111.2(3)
N8	GA2	C21	114.5(2)	S10	C9	N11	127.9(3)
C20	GA2	C21	123.5(2)	N8	C9	N11	120.9(3)
C2	S1	C5	92.0(2)	N11	C12	C13	119.6(4)
GA2	S10	C9	78.6(1)	N11	C12	C17	120.6(4)
GA1	N7	N8	110.9(2)	C13	C12	C17	119.8(4)
GA1	N7	C6	133.3(3)	C12	C13	C14	119.5(4)
N8	N7	C6	115.7(3)	C13	C14	C15	120.3(4)
GA2	N8	N7	145.0(2)	C14	C15	C16	119.7(4)
GA2	N8	C9	101.0(2)	C15	C16	C17	120.0(4)
N7	N8	C9	114.0(3)	C12	C17	C16	120.7(4)
GA1	N11	C9	114.7(2)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

INTRA

GA1	N7	1	2.1086	0.0029	1	1
GA1	N11	1	1.9683	0.0029	1	1
GA1	C18	1	1.9562	0.0045	1	1
GA1	C19	1	1.9594	0.0044	1	1
GA2	S10	1	2.4073	0.0010	1	1
GA2	N8	1	2.0556	0.0029	1	1
GA2	C20	1	1.9503	0.0044	1	1
GA2	C21	1	1.9358	0.0049	1	1
S1	C2	1	1.6961	0.0045	1	1
S1	C5	1	1.7074	0.0043	1	1
S10	C9	1	1.7269	0.0036	1	1
N7	N8	1	1.3844	0.0038	1	1
N7	C6	1	1.3019	0.0044	1	1
N8	C9	1	1.3576	0.0043	1	1
N11	C9	1	1.3173	0.0043	1	1
N11	C12	1	1.4355	0.0045	1	1
C2	C3	1	1.3311	0.0069	1	1
C3	C4	1	1.3988	0.0062	1	1
C4	C5	1	1.3800	0.0054	1	1
C5	C6	1	1.4359	0.0052	1	1
C12	C13	1	1.3763	0.0055	1	1
C12	C17	1	1.3645	0.0055	1	1
C13	C14	1	1.3912	0.0061	1	1
C14	C15	1	1.3707	0.0071	1	1
C15	C16	1	1.3722	0.0069	1	1
C16	C17	1	1.3762	0.0061	1	1

INTRA

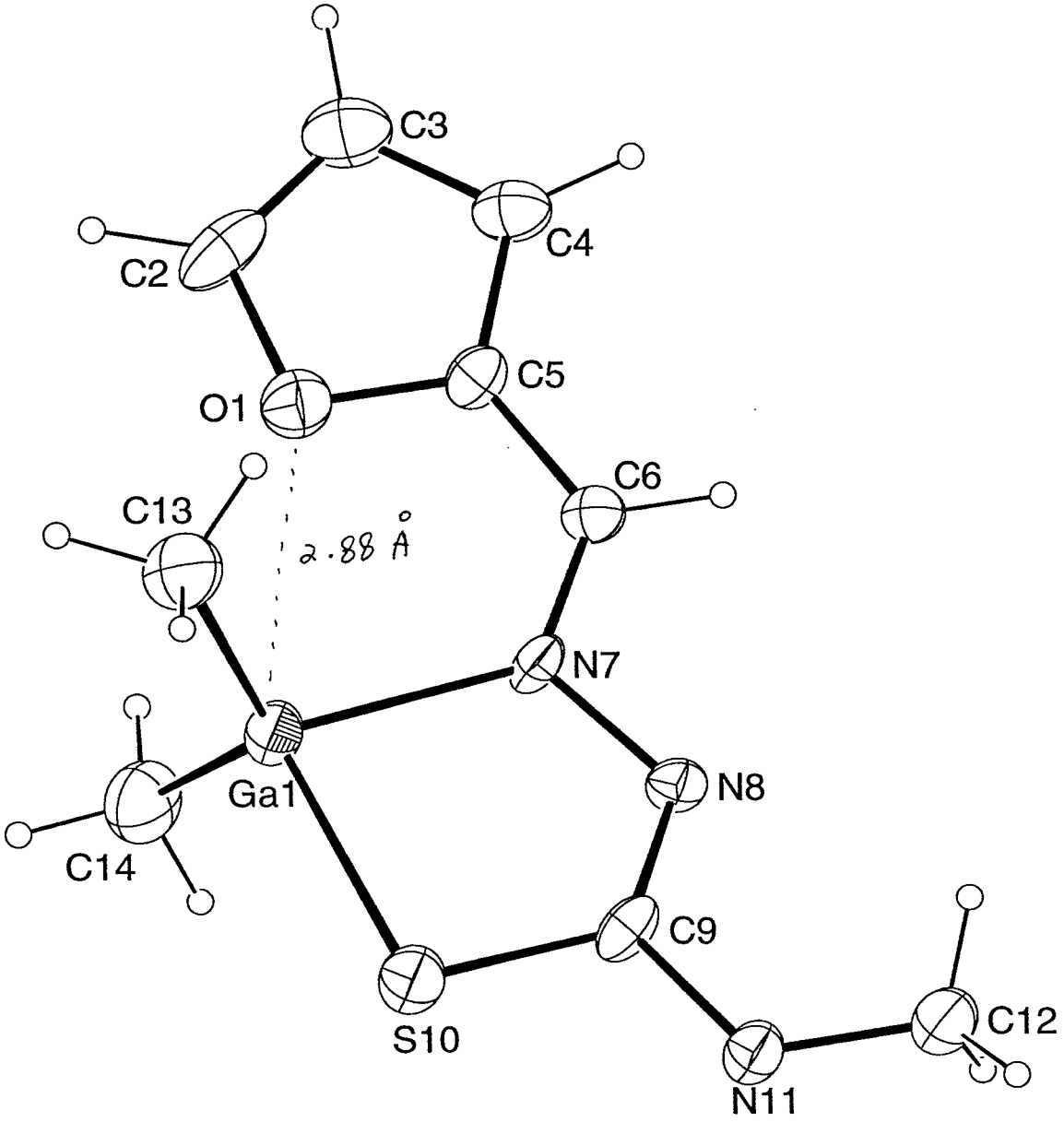
N7	GA1	N11	79.2098	0.1134
N7	GA1	C18	109.4273	0.1609
N7	GA1	C19	109.9014	0.1618
N11	GA1	C18	112.0523	0.1678
N11	GA1	C19	109.7478	0.1519
C18	GA1	C19	126.4932	0.1943
S10	GA2	N8	69.2741	0.0794
S10	GA2	C20	112.8224	0.1286
S10	GA2	C21	112.4237	0.1435
N8	GA2	C20	111.9928	0.1700
N8	GA2	C21	114.4823	0.1787
C20	GA2	C21	123.4656	0.2059
C2	S1	C5	91.9540	0.2264
GA2	S10	C9	78.5680	0.1214
GA1	N7	N8	110.9276	0.2004
GA1	N7	C6	133.3324	0.2536
N8	N7	C6	115.6553	0.2989
GA2	N8	N7	144.9942	0.2209
GA2	N8	C9	100.9556	0.2129
N7	N8	C9	114.0490	0.2834
GA1	N11	C9	114.7456	0.2407
GA1	N11	C12	124.9779	0.2338
C9	N11	C12	120.2515	0.3064
S1	C2	C3	111.6435	0.3483
C2	C3	C4	114.2557	0.4449
C3	C4	C5	111.2624	0.4256
S1	C5	C4	110.8741	0.3055
S1	C5	C6	125.7517	0.3012
C4	C5	C6	123.3654	0.3802
N7	C6	C5	125.6046	0.3456
S10	C9	N8	111.1705	0.2542
S10	C9	N11	127.9179	0.2808
N8	C9	N11	120.8797	0.3196
N11	C12	C13	119.5854	0.3590
N11	C12	C17	120.5537	0.3531
C13	C12	C17	119.7927	0.3698
C12	C13	C14	119.5002	0.4216
C13	C14	C15	120.2623	0.4335
C14	C15	C16	119.6960	0.4158
C15	C16	C17	120.0104	0.4472
C12	C17	C16	120.7264	0.4179

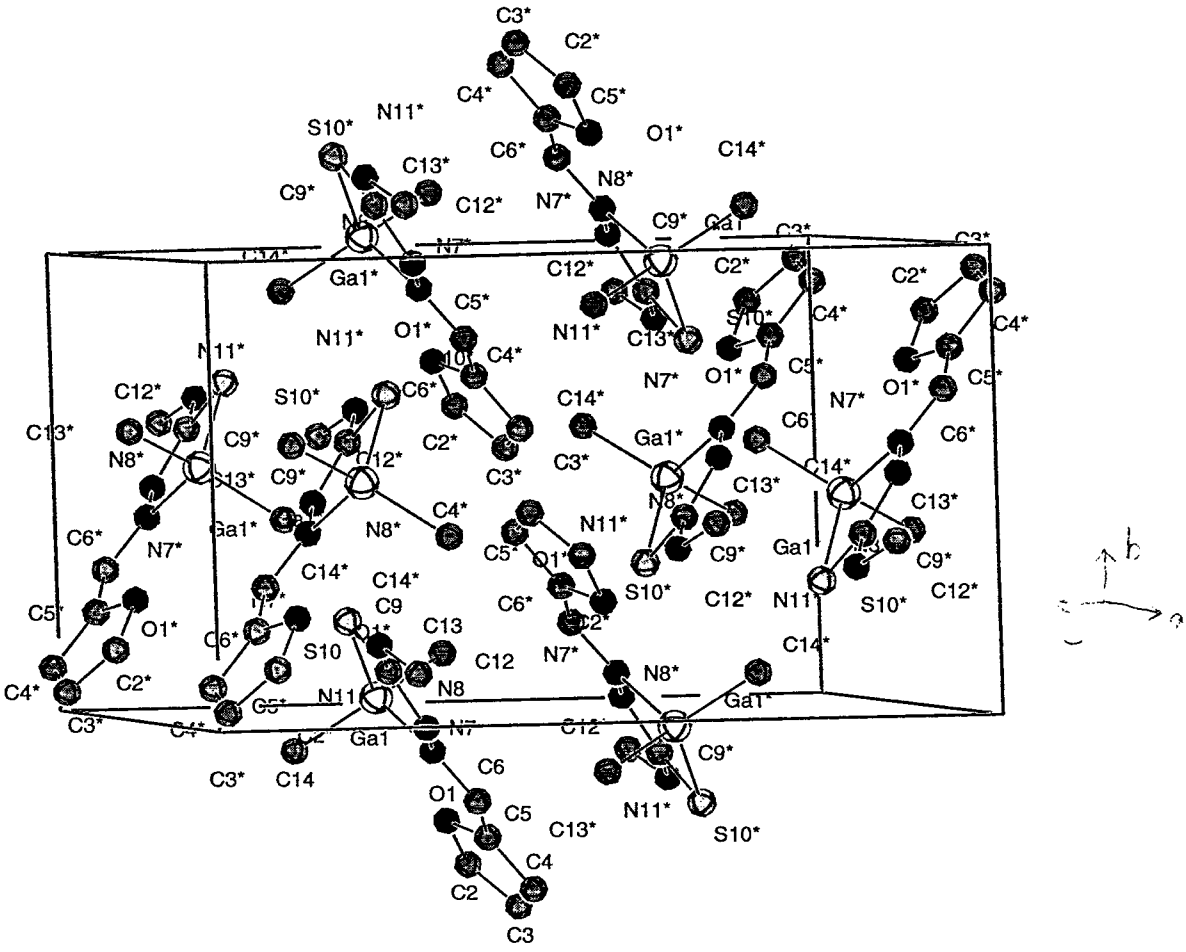
INTRA

C2	H2	1	0.9430	0.0000	1	1
C3	H3	1	0.9564	0.0000	1	1
C4	H4	1	0.9266	0.0000	1	1
C6	H6	1	0.9524	0.0000	1	1
C13	H13	1	0.9441	0.0000	1	1
C14	H14	1	0.9542	0.0000	1	1
C15	H15	1	0.9500	0.0000	1	1
C16	H16	1	0.9476	0.0000	1	1
C17	H17	1	0.9393	0.0000	1	1
C18	H18a	1	0.9464	0.0000	1	1
C18	H18b	1	0.9545	0.0000	1	1
C18	H18c	1	0.9429	0.0000	1	1
C19	H19a	1	0.9521	0.0000	1	1
C19	H19b	1	0.9460	0.0000	1	1
C19	H19c	1	0.9470	0.0000	1	1
C20	H20b	1	0.9505	0.0000	1	1
C20	H20a	1	0.9454	0.0000	1	1
C20	H20c	1	0.9463	0.0000	1	1
C21	H21a	1	0.9595	0.0000	1	1
C21	H21b	1	0.9491	0.0000	1	1
C21	H21c	1	0.9461	0.0000	1	1

INTRA

S1	C2	H2	124.4595	0.0000
C3	C2	H2	123.8956	0.0000
C2	C3	H3	122.5736	0.0000
C4	C3	H3	123.1703	0.0000
C3	C4	H4	123.3917	0.0000
C5	C4	H4	125.3229	0.0000
N7	C6	H6	117.0974	0.0000
C5	C6	H6	117.2967	0.0000
C12	C13	H13	120.2606	0.0000
C14	C13	H13	120.2387	0.0000
C13	C14	H14	119.6104	0.0000
C15	C14	H14	120.1264	0.0000
C14	C15	H15	120.0890	0.0000
C16	C15	H15	120.2150	0.0000
C15	C16	H16	119.6600	0.0000
C17	C16	H16	120.3296	0.0000
C12	C17	H17	119.8432	0.0000
C16	C17	H17	119.4286	0.0000
GA1	C18	H18a	109.1941	0.0000
GA1	C18	H18b	108.7705	0.0000
GA1	C18	H18c	109.3660	0.0000
H18a	C18	H18b	109.3930	0.0000
H18a	C18	H18c	110.3941	0.0000
H18b	C18	H18c	109.6964	0.0000
GA1	C19	H19a	108.9864	0.0000
GA1	C19	H19b	109.3133	0.0000
GA1	C19	H19c	109.2638	0.0000
H19a	C19	H19b	109.6310	0.0000
H19a	C19	H19c	109.5480	0.0000
H19b	C19	H19c	110.0784	0.0000
GA2	C20	H20b	108.8495	0.0000
GA2	C20	H20a	109.1222	0.0000
GA2	C20	H20c	109.0784	0.0000
H20b	C20	H20a	109.8244	0.0000
H20b	C20	H20c	109.7498	0.0000
H20a	C20	H20c	110.1902	0.0000
GA2	C21	H21a	109.3151	0.0000
GA2	C21	H21b	109.8563	0.0000
GA2	C21	H21c	110.0146	0.0000
H21a	C21	H21b	108.7442	0.0000
H21a	C21	H21c	108.9960	0.0000
H21b	C21	H21c	109.8887	0.0000


C3
C4
C2
C5
O1
C6
C13
2.88 Å
N7
Ga1
N8
C14
C9
S10
C12
N11



Positional parameters and B(eq) for $(GaMe_2)[OC_4H_3CHNNC(S)NHCH_3]$

atom	x	y	z	B(eq)
Ga1	0.3355(1)	0.0298(1)	0.65664(9)	3.14(3)
S10	0.5073(3)	0.2067(3)	0.7275(2)	3.88(7)
O1	0.2462(7)	-0.2481(8)	0.5502(5)	4.1(2)
N7	0.4918(7)	-0.0809(8)	0.6187(6)	2.7(2)
N8	0.6265(7)	-0.0230(9)	0.6546(5)	2.5(2)
N11	0.7654(8)	0.1661(9)	0.7423(6)	3.2(2)
C2	0.147(1)	-0.351(1)	0.5022(10)	5.0(3)
C3	0.190(1)	-0.442(1)	0.4469(9)	4.7(3)
C4	0.325(1)	-0.396(1)	0.4565(8)	3.7(3)
C5	0.3567(9)	-0.279(1)	0.5210(7)	3.0(2)
C6	0.4803(9)	-0.193(1)	0.5599(7)	2.8(2)
C9	0.6390(9)	0.103(1)	0.7042(7)	3.0(2)
C12	0.884(1)	0.109(1)	0.7181(8)	3.8(3)
C13	0.201(1)	0.117(1)	0.5396(9)	4.7(3)
C14	0.291(1)	-0.086(1)	0.7562(9)	5.0(3)
H2	0.0542	-0.3543	0.5077	5.8264
H3	0.1378	-0.5250	0.4081	5.5655
H4	0.3856	-0.4401	0.4230	4.6824
H6	0.5604	-0.2215	0.5409	3.2531
H12a	0.9438	0.1897	0.7130	4.4768
H12b	0.9361	0.0398	0.7671	4.4768
H12c	0.8550	0.0559	0.6568	4.4768
H13a	0.2122	0.2237	0.5367	5.4832
H13b	0.2090	0.0722	0.4816	5.4832
H13c	0.1073	0.0983	0.5401	5.4832
H14a	0.2196	-0.0351	0.7747	5.7193
H14b	0.2591	-0.1838	0.7329	5.7193
H14c	0.3702	-0.0948	0.8129	5.7193

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
GA1	S10	2.328(3)	N7	C6	1.29(1)
GA1	N7	2.089(7)	N8	C9	1.31(1)
GA1	C13	1.96(1)	N11	C9	1.35(1)
GA1	C14	1.93(1)	N11	C12	1.45(1)
S10	C9	1.74(1)	C2	C3	1.31(2)
O1	C2	1.37(1)	C3	C4	1.40(2)
O1	C5	1.35(1)	C4	C5	1.36(1)
N7	N8	1.40(1)	C5	C6	1.42(1)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
S10	GA1	N7	84.1(2)	C9	N11	C12	121.3(9)
S10	GA1	C13	109.8(4)	O1	C2	C3	112(1)
S10	GA1	C14	110.4(4)	C2	C3	C4	106(1)
N7	GA1	C13	109.8(4)	C3	C4	C5	108(1)
N7	GA1	C14	109.2(4)	O1	C5	C4	108.9(9)
C13	GA1	C14	125.7(5)	O1	C5	C6	119.7(9)
GA1	S10	C9	94.8(3)	C4	C5	C6	131(1)
C2	O1	C5	105.6(9)	N7	C6	C5	123.5(9)
GA1	N7	N8	118.3(6)	S10	C9	N8	127.2(7)
GA1	N7	C6	128.1(6)	S10	C9	N11	113.7(8)
N8	N7	C6	113.4(7)	N8	C9	N11	119.1(9)
N7	N8	C9	115.2(7)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.