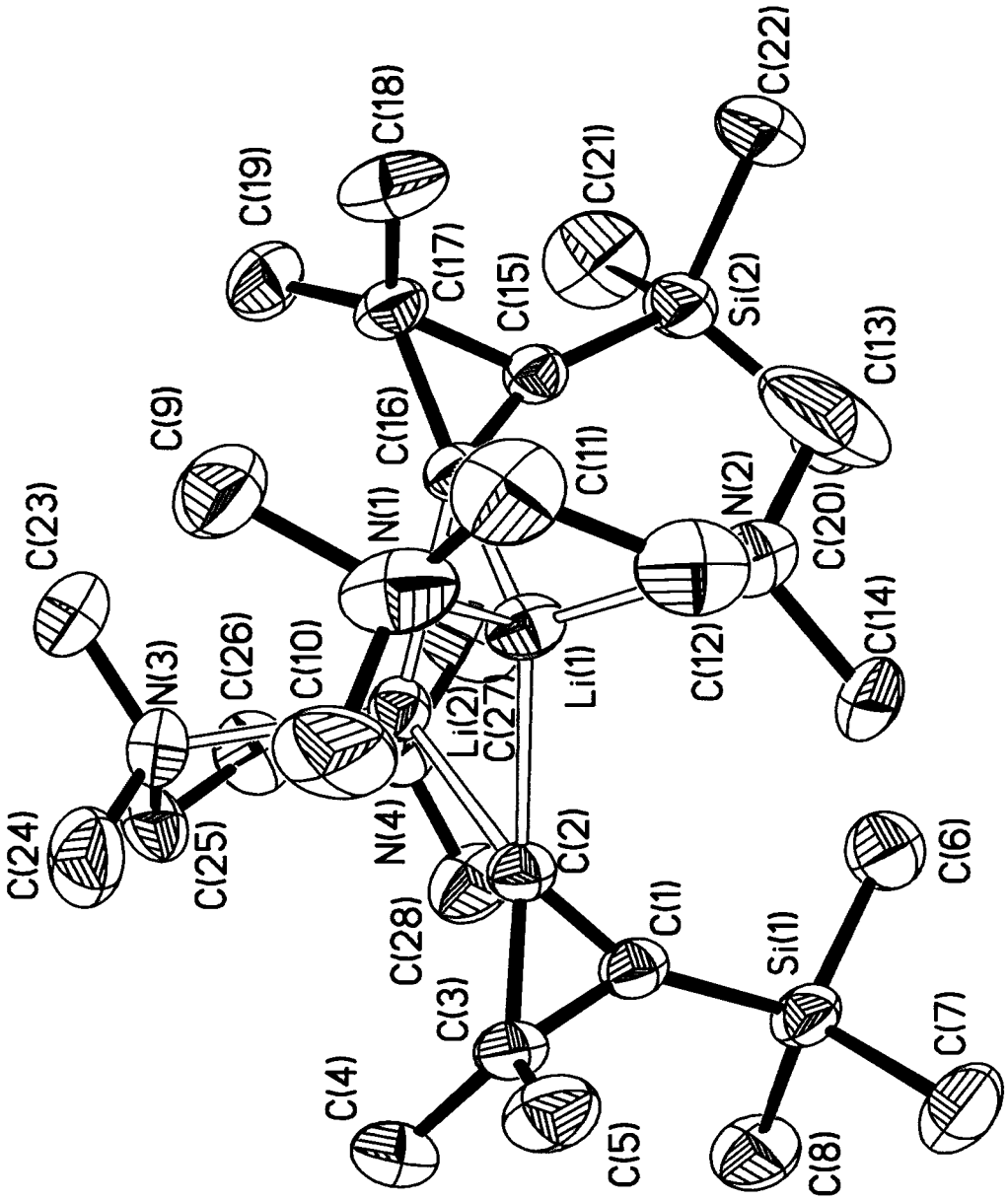
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(5), 1086-1091, DOI:10.1021/ja9521280

J1091-1



picture for suppl. material

Table 2. Crystal data and structure refinement for 2

J1091-2

Identification code	klas
Empirical formula	$C_{28}H_{62}Li_2N_4Si_2$
Formula weight	524.88
Temperature	153(2) K
Wavelength	71.073 pm
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 1879.9(2) pm alpha = 90° b = 1035.0(2) pm beta = 113.198(9)° c = 2045.5(2) pm gamma = 90°
Volume, Z	3.6580(8) nm^3, 4
Density (calculated)	0.953 Mg/m^3
Absorption coefficient	0.116 mm^{-1}
F(000)	1168
Crystal size	.6 x .6 x .8 mm
θ range for data collection	4.04 to 27.58°
Limiting indices	$-24 \le h \le 22$, $-8 \le k \le 13$, $0 \le l \le 26$
Reflections collected	9413
Independent reflections	8446 (R_{int} = 0.0700)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8446 / 85 / 431
Goodness-of-fit on F^2	1.022
Final R indices [I>2σ(I)]	R1 = 0.0491, wR2 = 0.1192
R indices (all data)	R1 = 0.0806, wR2 = 0.1381
Largest diff. peak and hole	345 and -278 $e.nm^{-3}$

J1091-3

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Li(1)	7872(2)	4309(3)	5359(1)	35(1)
C(1)	6981(1)	4662(2)	3633(1)	34(1)
C(2)	7573(1)	4206(2)	4197(1)	32(1)
C(3)	7745(1)	4858(2)	3587(1)	36(1)
C(4)	7951(1)	4052(2)	3070(1)	54(1)
C(5)	8090(1)	6195(2)	3677(1)	53(1)
Si(1)	5967(1)	4997(1)	3101(1)	39(1)
C(6)	5325(1)	4428(2)	3541(1)	54(1)
C(7)	5841(1)	6771(2)	2935(1)	63(1)
C(8)	5676(1)	4193(3)	2215(1)	61(1)
C(9)	9594(3)	4043(7)	6408(3)	65(2)
C(10)	9388(9)	5605(21)	5501(7)	78(4)
N(1)	9006(1)	5154(2)	5954(1)	60(1)
C(11)	8888(3)	5995(6)	6396(3)	62(2)
C(13)	6983(3)	5659(3)	6109(2)	142(2)
C(14)	6943(10)	6725(13)	5052(8)	56(4)
N(2)	7415(1)	5968(2)	5686(1)	50(1)
C(12)	8187(4)	6802(6)	5979(4)	58(2)
C(9′)	9425(4)	4764(7)	6654(3)	77(2)
C(10′)	9423(7)	5329(19)	5526(6)	85(4)
C(11′)	8684(4)	6606(6)	6020(4)	91(3)
C(12′)	8008(4)	6563(6)	6224(3)	75(2)
C(14′)	6913(9)	6753(14)	5121(8)	60(4)
Li(2)	7626(2)	2277(3)	4674(1)	32(1)
C(15)	7091(1)	2125(2)	6003(1)	33(1)
C(16)	7616(1)	2450(2)	5747(1)	31(1)
C(17)	7889(1)	1742(2)	6478(1)	39(1)
C(18)	8306(1)	2467(3)	7165(1)	62(1)
C(19)	8104(1)	329(2)	6547(1)	59(1)
Si(2)	6145(1)	1945(1)	6038(1)	49(1)
C(20)	5336(1)	2718(3)	5287(1)	74(1)
C(21)	5936(2)	187(3)	6060(2)	86(1)
C(22)	6196(2)	2677(3)	6887(1)	81(1)
C(27)	6365(2)	276(2)	4344(1)	68(1)
C(28)	6441(1)	1138(2)	3300(1)	59(1)
N(4)	6894(1)	751(1)	4031(1)	40(1)
C(26)	7424(3)	-262(6)	4075(4)	54(2)
C(25)	8153(2)	207(3)	4044(2)	48(1)
N(3)	8572(1)	1135(2)	4662(1)	48(1)
C(23)	8944(3)	423(6)	5296(2)	72(1)
C(24)	9139(4)	1825(7)	4461(4)	65(2)
C(26′)	7483(6)	-209(13)	3996(8)	87(7)
C(25′)	8250(4)	-96(6)	4602(4)	68(3)
C(24′)	8934(7)	1613(19)	4238(7)	100(7)
C(23′)	9211(4)	1273(10)	5455(3)	62(2)

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Table 4. Selected bond lengths [pm] and angles [°] for 2.

Li(1)-N(2)	214.1(3)	Li(1)-N(1)	217.9(3)
Li(1)-C(16)	220.5(3)	Li(1)-C(2)	221.9(3)
C(1)-C(2)	133.3(2)	C(1)-C(3)	148.9(2)
C(1)-Si(1)	181.8(2)	C(2)-C(3)	156.1(2)
C(2)-Li(2)	220.7(3)	Li(2)-N(3)	214.4(3)
Li(2)-N(4)	216.6(3)	Li(2)-C(16)	220.9(3)
C(15)-C(16)	132.9(2)	C(15)-C(17)	148.5(2)
C(15)-Si(2)	181.8(2)	C(16)-C(17)	155.9(2)

N(2)-Li(1)-N(1)	85.86(12)	N(2)-Li(1)-C(16)	114.60(14)
N(1)-Li(1)-C(16)	116.91(14)	N(2)-Li(1)-C(2)	114.19(14)
N(1)-Li(1)-C(2)	113.40(14)	C(16)-Li(1)-C(2)	110.16(13)
C(2)-C(1)-C(3)	66.88(12)	C(2)-C(1)-Si(1)	154.90(14)
C(3)-C(1)-Si(1)	138.23(12)	C(1)-C(2)-C(3)	61.34(11)
C(1)-C(2)-Li(2)	125.47(14)	C(3)-C(2)-Li(2)	139.21(13)
C(1)-C(2)-Li(1)	133.0(2)	C(3)-C(2)-Li(1)	142.26(14)
Li(2)-C(2)-Li(1)	67.76(11)	C(1)-C(3)-C(5)	119.7(2)
C(1)-C(3)-C(4)	119.3(2)	C(5)-C(3)-C(4)	112.1(2)
C(1)-C(3)-C(2)	51.78(10)	C(5)-C(3)-C(2)	120.9(2)
C(4)-C(3)-C(2)	120.8(2)	C(1)-Si(1)-C(6)	112.17(9)
C(1)-Si(1)-C(7)	108.93(10)	N(3)-Li(2)-N(4)	85.53(11)
N(3)-Li(2)-C(2)	112.76(14)	N(4)-Li(2)-C(2)	118.91(13)
N(3)-Li(2)-C(16)	112.83(13)	N(4)-Li(2)-C(16)	114.25(14)
C(2)-Li(2)-C(16)	110.46(13)	C(16)-C(15)-C(17)	67.04(12)
C(16)-C(15)-Si(2)	158.66(14)	C(17)-C(15)-Si(2)	134.28(12)
C(15)-C(16)-C(17)	61.26(11)	C(15)-C(16)-Li(1)	131.5(2)
C(17)-C(16)-Li(1)	136.01(13)	C(15)-C(16)-Li(2)	131.90(14)
C(17)-C(16)-Li(2)	141.82(14)	Li(1)-C(16)-Li(2)	67.96(11)
C(15)-C(17)-C(19)	119.0(2)	C(15)-C(17)-C(18)	119.7(2)
C(19)-C(17)-C(18)	111.9(2)	C(15)-C(17)-C(16)	51.71(10)
C(19)-C(17)-C(16)	121.4(2)	C(18)-C(17)-C(16)	120.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Bond lengths [pm] and angles [°] for 2. J1091-5

Li(1)-N(2)	214.1(3)	Li(1)-N(1)	217.9(3)
Li(1)-C(16)	220.5(3)	Li(1)-C(2)	221.9(3)
Li(1)-Li(2)	246.7(4)	C(1)-C(2)	133.3(2)
C(1)-C(3)	148.9(2)	C(1)-Si(1)	181.8(2)
C(2)-C(3)	156.1(2)	C(2)-Li(2)	220.7(3)
C(3)-C(5)	150.9(3)	C(3)-C(4)	151.2(3)
Si(1)-C(6)	186.2(2)	Si(1)-C(7)	186.6(2)
Si(1)-C(8)	186.9(2)	C(9)-N(1)	161.2(6)
C(10)-N(1)	145.5(10)	N(1)-C(11)	133.4(5)
N(1)-C(9′)	139.5(5)	N(1)-C(10′)	139.8(10)
N(1)-C(11′)	164.5(7)	C(11)-C(12)	150.9(10)
C(13)-N(2)	143.7(3)	C(14)-N(2)	147.6(10)
N(2)-C(12′)	136.6(6)	N(2)-C(14′)	142.5(10)
N(2)-C(12)	158.9(7)	C(11′)-C(12′)	148.8(11)
Li(2)-N(3)	214.4(3)	Li(2)-N(4)	216.6(3)
Li(2)-C(16)	220.9(3)	Li(2)-C(25′)	275.1(7)
C(15)-C(16)	132.9(2)	C(15)-C(17)	148.5(2)
C(15)-Si(2)	181.8(2)	C(16)-C(17)	155.9(2)
C(17)-C(19)	150.8(3)	C(17)-C(18)	151.1(3)
Si(2)-C(22)	186.3(2)	Si(2)-C(20)	186.3(2)
Si(2)-C(21)	186.5(3)	C(27)-N(4)	146.5(3)
C(28)-N(4)	145.5(2)	N(4)-C(26)	142.5(6)
N(4)-C(26′)	150.9(11)	C(26)-C(25)	147.9(6)
C(25)-N(3)	153.5(4)	N(3)-C(24′)	138.8(11)
N(3)-C(25′)	139.5(7)	N(3)-C(23)	141.4(4)
N(3)-C(24)	147.0(6)	N(3)-C(23′)	160.0(7)
C(26′)-C(25′)	149.1(13)		

N(2)-Li(1)-N(1)	85.86(12)	N(2)-Li(1)-C(16)	114.60(14)
N(1)-Li(1)-C(16)	116.91(14)	N(2)-Li(1)-C(2)	114.19(14)
N(1)-Li(1)-C(2)	113.40(14)	C(16)-Li(1)-C(2)	110.16(13)
N(2)-Li(1)-Li(2)	148.5(2)	N(1)-Li(1)-Li(2)	125.6(2)
C(16)-Li(1)-Li(2)	56.10(10)	C(2)-Li(1)-Li(2)	55.88(10)
C(2)-C(1)-C(3)	66.88(12)	C(2)-C(1)-Si(1)	154.90(14)
C(3)-C(1)-Si(1)	138.23(12)	C(1)-C(2)-C(3)	61.34(11)
C(1)-C(2)-Li(2)	125.47(14)	C(3)-C(2)-Li(2)	139.21(13)
C(1)-C(2)-Li(1)	133.0(2)	C(3)-C(2)-Li(1)	142.26(14)
Li(2)-C(2)-Li(1)	67.76(11)	C(1)-C(3)-C(5)	119.7(2)
C(1)-C(3)-C(4)	119.3(2)	C(5)-C(3)-C(4)	112.1(2)
C(1)-C(3)-C(2)	51.78(10)	C(5)-C(3)-C(2)	120.9(2)
C(4)-C(3)-C(2)	120.8(2)	C(1)-Si(1)-C(6)	112.17(9)
C(1)-Si(1)-C(7)	108.93(10)	C(6)-Si(1)-C(7)	109.80(11)
C(1)-Si(1)-C(8)	109.48(9)	C(6)-Si(1)-C(8)	109.25(11)
C(7)-Si(1)-C(8)	107.08(12)	C(9′)-N(1)-C(10′)	116.8(6)
C(11)-N(1)-C(10)	118.5(9)	C(11)-N(1)-C(9)	109.5(4)
C(10)-N(1)-C(9)	101.3(7)	C(9′)-N(1)-C(11′)	104.9(4)
C(10′)-N(1)-C(11′)	104.3(8)	C(11)-N(1)-Li(1)	104.7(2)
C(9′)-N(1)-Li(1)	119.4(3)	C(10′)-N(1)-Li(1)	111.7(6)
C(10)-N(1)-Li(1)	113.1(7)	C(9)-N(1)-Li(1)	109.5(3)
C(11′)-N(1)-Li(1)	95.9(2)	N(1)-C(11)-C(12)	108.7(5)
C(12′)-N(2)-C(14′)	117.8(7)	C(13)-N(2)-C(14)	111.0(9)
C(13)-N(2)-C(12)	122.8(3)	C(14)-N(2)-C(12)	100.8(7)
C(12′)-N(2)-Li(1)	108.3(3)	C(14′)-N(2)-Li(1)	115.0(8)
C(13)-N(2)-Li(1)	113.7(2)	C(14)-N(2)-Li(1)	109.2(8)
C(12)-N(2)-Li(1)	97.8(3)	C(11)-C(12)-N(2)	112.2(5)
C(12′)-C(11′)-N(1)	112.2(5)	N(2)-C(12′)-C(11′)	107.6(6)
N(3)-Li(2)-N(4)	85.53(11)	N(3)-Li(2)-C(2)	112.76(14)
N(4)-Li(2)-C(2)	118.91(13)	N(3)-Li(2)-C(16)	112.83(13)
N(4)-Li(2)-C(16)	114.25(14)	C(2)-Li(2)-C(16)	110.46(13)

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N(3)-Li(2)-Li(1)	120.40(14)	N(4)-Li(2)-Li(1)	153.9(2)
C(2)-Li(2)-Li(1)	56.36(10)	C(16)-Li(2)-Li(1)	55.94(10)
N(3)-Li(2)-C(25')	30.0(2)	N(4)-Li(2)-C(25')	59.9(2)
C(2)-Li(2)-C(25')	136.9(2)	C(16)-Li(2)-C(25')	107.2(2)
Li(1)-Li(2)-C(25')	143.4(2)	C(16)-C(15)-C(17)	67.04(12)
C(16)-C(15)-Si(2)	158.66(14)	C(17)-C(15)-Si(2)	134.28(12)
C(15)-C(16)-C(17)	61.26(11)	C(15)-C(16)-Li(1)	131.5(2)
C(17)-C(16)-Li(1)	136.01(13)	C(15)-C(16)-Li(2)	131.90(14)
C(17)-C(16)-Li(2)	141.82(14)	Li(1)-C(16)-Li(2)	67.96(11)
C(15)-C(17)-C(19)	119.0(2)	C(15)-C(17)-C(18)	119.7(2)
C(19)-C(17)-C(18)	111.9(2)	C(15)-C(17)-C(16)	51.71(10)
C(19)-C(17)-C(16)	121.4(2)	C(18)-C(17)-C(16)	120.8(2)
C(15)-Si(2)-C(22)	107.67(11)	C(15)-Si(2)-C(20)	114.61(10)
C(22)-Si(2)-C(20)	108.63(12)	C(15)-Si(2)-C(21)	108.70(11)
C(22)-Si(2)-C(21)	107.9(2)	C(20)-Si(2)-C(21)	109.11(14)
C(26)-N(4)-C(28)	112.3(4)	C(26)-N(4)-C(27)	107.7(3)
C(28)-N(4)-C(27)	108.6(2)	C(28)-N(4)-C(26')	106.0(6)
C(27)-N(4)-C(26')	115.9(6)	C(26)-N(4)-Li(2)	103.7(3)
C(28)-N(4)-Li(2)	113.44(14)	C(27)-N(4)-Li(2)	110.93(14)
C(26')-N(4)-Li(2)	101.9(5)	N(4)-C(26)-C(25)	113.1(4)
C(26)-C(25)-N(3)	110.7(4)	C(24')-N(3)-C(25')	125.0(8)
C(23)-N(3)-C(24)	111.0(3)	C(23)-N(3)-C(25)	109.7(3)
C(24)-N(3)-C(25)	105.5(3)	C(24')-N(3)-C(23')	104.1(6)
C(25')-N(3)-C(23')	107.2(5)	C(24')-N(3)-Li(2)	115.1(7)
C(25')-N(3)-Li(2)	99.9(3)	C(23)-N(3)-Li(2)	112.9(2)
C(24)-N(3)-Li(2)	115.6(3)	C(25)-N(3)-Li(2)	101.3(2)
C(23')-N(3)-Li(2)	103.5(3)	C(25')-C(26')-N(4)	113.4(9)
N(3)-C(25')-C(26')	112.8(7)	N(3)-C(25')-Li(2)	50.1(2)
C(26')-C(25')-Li(2)	79.7(5)		

Symmetry transformations used to generate equivalent atoms:

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Table 6. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 2.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Li(1)	42(2)	31(1)	27(1)	-3(1)	8(1)	-6(1)
C(1)	38(1)	35(1)	27(1)	2(1)	11(1)	2(1)
C(2)	37(1)	31(1)	26(1)	0(1)	12(1)	0(1)
C(3)	39(1)	42(1)	29(1)	7(1)	14(1)	2(1)
C(4)	60(1)	69(1)	39(1)	6(1)	27(1)	6(1)
C(5)	54(1)	51(1)	51(1)	14(1)	20(1)	-5(1)
Si(1)	35(1)	45(1)	31(1)	7(1)	6(1)	4(1)
C(6)	49(1)	58(1)	56(1)	2(1)	22(1)	-1(1)
C(7)	55(1)	56(1)	69(1)	23(1)	17(1)	13(1)
C(8)	54(1)	84(2)	32(1)	1(1)	3(1)	2(1)
C(9)	47(3)	84(5)	57(3)	18(3)	12(2)	9(3)
C(10)	61(6)	108(9)	80(7)	25(5)	42(6)	-18(5)
N(1)	49(1)	77(1)	41(1)	0(1)	6(1)	-27(1)
C(11)	55(3)	63(4)	50(3)	-21(3)	3(2)	-19(3)
C(13)	304(6)	60(2)	157(3)	29(2)	192(4)	57(3)
C(14)	74(8)	42(6)	53(6)	17(5)	27(5)	33(5)
N(2)	81(1)	30(1)	36(1)	-3(1)	18(1)	7(1)
C(12)	85(4)	33(3)	55(4)	-13(3)	27(4)	-16(3)
C(9')	77(4)	79(4)	54(3)	12(3)	3(3)	2(3)
C(10')	48(5)	113(8)	69(6)	21(5)	-2(4)	-31(4)
C(11')	80(4)	43(3)	101(5)	3(3)	-19(4)	-28(3)
C(12')	109(5)	33(3)	49(3)	-13(2)	-7(3)	7(3)
C(14')	62(6)	71(7)	44(4)	-13(4)	18(4)	10(5)
Li(2)	33(1)	31(1)	32(1)	-3(1)	12(1)	2(1)
C(15)	38(1)	30(1)	30(1)	1(1)	14(1)	2(1)
C(16)	36(1)	28(1)	28(1)	2(1)	11(1)	1(1)
C(17)	41(1)	41(1)	32(1)	11(1)	12(1)	2(1)
C(18)	65(1)	78(2)	32(1)	7(1)	6(1)	-13(1)
C(19)	66(1)	53(1)	62(1)	27(1)	29(1)	20(1)
Si(2)	40(1)	70(1)	43(1)	9(1)	22(1)	4(1)
C(20)	47(1)	116(2)	58(1)	10(1)	19(1)	18(1)
C(21)	70(2)	92(2)	104(2)	18(2)	41(2)	-27(2)
C(22)	77(2)	128(3)	52(1)	12(2)	42(1)	28(2)
C(27)	87(2)	56(1)	72(2)	-21(1)	44(1)	-28(1)
C(28)	65(1)	55(1)	44(1)	-6(1)	6(1)	0(1)
N(4)	48(1)	32(1)	38(1)	-7(1)	14(1)	1(1)
C(26)	62(4)	36(3)	65(4)	-13(2)	26(3)	-8(2)
C(25)	56(2)	42(2)	54(2)	-6(1)	30(2)	11(1)
N(3)	40(1)	50(1)	52(1)	7(1)	17(1)	15(1)
C(23)	56(2)	95(4)	61(2)	26(3)	17(2)	29(2)
C(24)	39(3)	70(3)	85(4)	12(3)	23(3)	4(2)
C(26')	92(11)	74(10)	59(7)	-33(6)	-8(6)	65(8)
C(25')	76(5)	43(4)	62(5)	-10(3)	2(4)	29(3)
C(24')	43(7)	200(18)	68(7)	45(9)	34(6)	47(8)
C(23')	43(4)	90(6)	46(4)	2(4)	9(3)	23(4)

Table 7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 2.

	x	y	z	U(eq)
H(4A)	8515(1)	3987(11)	3238(4)	64
H(4B)	7742(7)	4461(7)	2600(2)	64
H(4C)	7730(7)	3185(5)	3037(5)	64
H(5A)	8654(1)	6130(2)	3842(7)	63
H(5B)	7959(6)	6673(5)	4028(5)	63
H(5C)	7881(6)	6651(5)	3221(2)	63
H(6A)	4783(1)	4542(12)	3216(3)	65
H(6B)	5429(6)	4932(9)	3974(4)	65
H(6C)	5425(6)	3512(4)	3663(6)	65
H(7A)	5307(3)	6951(3)	2608(6)	75
H(7B)	6198(6)	7073(3)	2725(7)	75
H(7C)	5951(8)	7223(2)	3386(2)	75
H(8A)	5144(3)	4440(12)	1912(3)	74
H(8B)	5706(8)	3254(3)	2279(1)	74
H(8C)	6025(5)	4465(11)	1990(4)	74
H(9A)	9671(18)	3415(21)	6083(3)	98
H(9B)	9378(11)	3605(25)	6713(15)	98
H(9C)	10092(8)	4434(8)	6704(16)	98
H(10A)	9400(25)	4905(23)	5183(18)	118
H(10B)	9918(13)	5871(49)	5797(7)	118
H(10C)	9102(18)	6342(33)	5218(20)	118
H(11A)	9348(3)	6558(6)	6613(3)	74
H(11B)	8804(3)	5527(6)	6781(3)	74
H(13A)	7306(7)	5146(30)	6521(10)	213
H(13B)	6521(11)	5162(30)	5822(6)	213
H(13C)	6826(19)	6459(3)	6271(16)	213
H(14A)	6509(18)	6197(22)	4741(15)	84
H(14B)	7262(11)	6985(46)	4795(19)	84
H(14C)	6743(29)	7497(30)	5200(8)	84
H(12A)	8263(4)	7213(6)	5575(4)	70
H(12B)	8133(4)	7497(6)	6289(4)	70
H(9'1)	9888(13)	5304(27)	6866(8)	116
H(9'2)	9579(21)	3858(14)	6660(3)	116
H(9'3)	9102(9)	4857(38)	6929(6)	116
H(10D)	9081(11)	5686(44)	5066(12)	127
H(10E)	9628(23)	4496(21)	5453(20)	127
H(10F)	9852(19)	5929(41)	5760(14)	127
H(11C)	9106(4)	7108(6)	6380(4)	110
H(11D)	8534(4)	7057(6)	5558(4)	110
H(12C)	8140(4)	6075(6)	6673(3)	90
H(12D)	7854(4)	7450(6)	6296(3)	90
H(14D)	7155(13)	6931(43)	4785(17)	89
H(14E)	6816(27)	7569(25)	5315(9)	89
H(14F)	6422(12)	6300(25)	4874(17)	89
H(18A)	8866(1)	2395(12)	7302(4)	75
H(18B)	8167(7)	2097(10)	7540(2)	75
H(18C)	8154(7)	3379(4)	7098(2)	75
H(19A)	8662(2)	241(2)	6680(7)	71
H(19B)	7825(6)	-106(3)	6092(2)	71
H(19C)	7962(8)	-66(4)	6915(5)	71
H(20A)	4853(2)	2612(14)	5357(5)	89
H(20B)	5285(6)	2307(11)	4839(2)	89
H(20C)	5446(5)	3640(4)	5269(5)	89

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H(21A)	5454(6)	77(3)	6132(10)	104
H(21B)	6362(5)	-226(4)	6452(6)	104
H(21C)	5882(11)	-213(5)	5609(4)	104
H(22A)	5725(5)	2461(14)	6961(5)	97
H(22B)	6240(10)	3618(4)	6864(4)	97
H(22C)	6648(6)	2338(13)	7283(2)	97
H(27A)	6000(7)	962(6)	4330(9)	102
H(27B)	6662(2)	20(17)	4839(3)	102
H(27C)	6079(8)	-472(11)	4073(6)	102
H(28A)	6066(7)	1801(12)	3293(1)	89
H(28B)	6166(8)	386(4)	3025(2)	89
H(28C)	6787(2)	1489(15)	3089(3)	89
H(26A)	7174(3)	-875(6)	3678(4)	65
H(26B)	7546(3)	-739(6)	4526(4)	65
H(25A)	8038(2)	658(3)	3586(2)	58
H(25B)	8494(2)	-537(3)	4068(2)	58
H(23A)	9213(15)	1018(6)	5688(4)	109
H(23B)	9319(13)	-172(23)	5236(6)	109
H(23C)	8558(3)	-71(24)	5402(9)	109
H(24A)	9430(12)	2434(20)	4838(8)	98
H(24B)	8869(4)	2299(24)	4017(9)	98
H(24C)	9497(11)	1201(7)	4394(15)	98
H(26C)	7280(6)	-1094(13)	3991(8)	104
H(26D)	7552(6)	-81(13)	3545(8)	104
H(25C)	8191(4)	-309(6)	5050(4)	82
H(25D)	8610(4)	-734(6)	4538(4)	82
H(24D)	9381(29)	1069(47)	4293(33)	149
H(24E)	9109(40)	2499(32)	4383(28)	149
H(24F)	8569(16)	1608(75)	3739(8)	149
H(23D)	9424(22)	2150(18)	5526(9)	93
H(23E)	9627(16)	648(36)	5529(9)	93
H(23F)	8973(8)	1104(50)	5795(3)	93