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OM961082W

Table 1. Crystal data and structure refinement for 1.

Identification code	saw56i
Empirical formula	$C_{12}H_{18}LiN_3$
Formula weight	211.23
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.138(10) Å α = 90.56(9)° b = 11.151(11) Å β = 100.55(8)° c = 22.14(3) Å γ = 112.24(8)°
Volume	2493(4) $Å^3$
Z	8
Density (calculated)	1.126 Mg/m^3
Absorption coefficient	0.067 mm^{-1}
F(000)	912
Crystal size	0.5 x 0.3 x 0.3 mm
θ range for data collection	3.58 to 25.15°
Index ranges	$-13 \leq h \leq 11$, $-13 \leq k \leq 13$, $0 \leq \ell \leq 26$
Reflections collected	15901
Independent reflections	8337 (R_{int} = 0.1007)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8328 / 0 / 589
Goodness-of-fit on F^2	1.035
Final R indices [$I>2\sigma(I)$]	R1 = 0.0623, wR2 = 0.1500
R indices (all data)	R1 = 0.0914, wR2 = 0.1750
Largest diff. peak and hole	0.425 and -0.261 $eÅ^{-3}$

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 U_{ij} tensor.

	x	y	z	U(eq)
Li(1)	9532(4)	2307(4)	2050(2)	24(1)
Li(2)	7759(4)	2377(4)	2693(2)	26(1)
Li(3)	7397(4)	234(4)	2008(2)	27(1)
Li(4)	9239(4)	1053(4)	3041(2)	28(1)
C(1)	7439(3)	1636(3)	4166(1)	36(1)
C(2)	7361(3)	2362(3)	4657(1)	43(1)
C(3)	6140(3)	2122(3)	4814(1)	43(1)
C(4)	5028(3)	1142(3)	4485(1)	42(1)
C(5)	5113(3)	393(3)	4003(1)	36(1)
C(6)	6328(3)	637(2)	3835(1)	29(1)
C(7)	6455(2)	-65(2)	3272(1)	27(1)
N(8)	7172(2)	491(2)	2903(1)	26(1)
N(9)	5538(2)	-1428(2)	3182(1)	33(1)
C(10)	5652(3)	-2192(3)	3708(1)	43(1)
C(11)	5506(3)	-2061(2)	2601(1)	35(1)
C(12)	4825(3)	-1578(3)	2060(1)	35(1)
N(13)	5532(2)	-1281(2)	1546(1)	32(1)
C(14)	5547(3)	-2471(3)	1268(2)	49(1)
C(15)	4848(3)	-718(3)	1075(1)	44(1)
C(16)	10876(3)	4066(3)	4375(1)	41(1)
C(17)	11484(4)	3986(3)	4966(1)	58(1)
C(18)	12719(5)	3926(3)	5074(2)	66(1)
C(19)	13343(4)	3942(4)	4588(2)	64(1)
C(20)	12738(3)	4037(3)	3992(2)	48(1)
C(21)	11488(3)	4086(2)	3877(1)	31(1)
C(22)	10741(2)	4010(2)	3225(1)	24(1)
N(23)	9821(2)	2974(2)	2973(1)	24(1)
N(24)	11257(2)	5176(2)	2926(1)	30(1)
C(25)	11964(3)	6443(3)	3269(1)	43(1)
C(26)	10553(3)	5188(3)	2308(1)	31(1)
C(27)	11160(3)	4953(3)	1776(1)	33(1)
N(28)	11249(2)	3668(2)	1736(1)	28(1)
C(29)	11287(3)	3308(3)	1106(1)	41(1)
C(30)	12475(3)	3712(3)	2136(1)	39(1)
C(31)	8770(3)	-2599(3)	1592(1)	35(1)
C(32)	8062(3)	-3519(3)	1099(1)	38(1)
C(33)	7927(3)	-3143(3)	505(1)	38(1)
C(34)	8487(3)	-1849(3)	410(1)	35(1)
C(35)	9185(3)	-925(3)	901(1)	31(1)
C(36)	9334(3)	-1281(2)	1504(1)	27(1)
C(37)	9921(2)	-254(2)	2043(1)	25(1)
N(38)	9318(2)	435(2)	2171(1)	25(1)
N(39)	11112(2)	-253(2)	2414(1)	33(1)
C(40)	12015(3)	-669(3)	2148(2)	44(1)
C(41)	11751(3)	737(3)	2928(1)	35(1)
C(42)	11504(3)	324(3)	3558(1)	36(1)
N(43)	10129(2)	-34(2)	3630(1)	32(1)
C(44)	10097(4)	185(3)	4277(1)	51(1)
C(45)	9340(3)	-1419(3)	3423(1)	40(1)
C(46)	7905(3)	3511(3)	320(1)	35(1)
C(47)	8480(3)	3543(3)	-187(1)	37(1)
C(48)	8701(3)	2481(3)	-377(1)	32(1)

C(49)	8358(3)	1391(3)	-53(1)	31(1)
C(50)	7811(3)	1368(2)	463(1)	28(1)
C(51)	7570(2)	2428(2)	660(1)	25(1)
C(52)	7091(2)	2435(2)	1259(1)	24(1)
N(53)	7611(2)	2130(2)	1752(1)	24(1)
N(54)	6059(2)	2937(2)	1207(1)	32(1)
C(55)	5005(3)	2571(3)	659(1)	45(1)
C(56)	5611(3)	2968(3)	1785(1)	34(1)
C(57)	6581(3)	4113(2)	2236(1)	30(1)
N(58)	6858(2)	3748(2)	2868(1)	29(1)
C(59)	5658(3)	3303(3)	3124(1)	42(1)
C(60)	7858(3)	4881(3)	3257(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

Li(1)-N(38)	2.035(5)	Li(1)-N(53)	2.052(5)
Li(1)-N(23)	2.094(5)	Li(1)-N(28)	2.180(5)
Li(1)-Li(3)	2.600(6)	Li(1)-Li(4)	2.619(6)
Li(1)-Li(2)	2.661(6)	Li(2)-N(8)	2.038(5)
Li(2)-N(53)	2.068(5)	Li(2)-N(23)	2.101(5)
Li(2)-N(58)	2.188(5)	Li(2)-Li(4)	2.624(6)
Li(2)-Li(3)	2.673(6)	Li(3)-N(38)	2.028(5)
Li(3)-N(8)	2.073(5)	Li(3)-N(53)	2.131(5)
Li(3)-N(13)	2.179(6)	Li(3)-Li(4)	2.664(7)
Li(4)-N(23)	2.005(5)	Li(4)-N(38)	2.067(5)
Li(4)-N(8)	2.105(5)	Li(4)-N(43)	2.149(5)
C(1)-C(2)	1.384(4)	C(1)-C(6)	1.384(4)
C(2)-C(3)	1.394(4)	C(3)-C(4)	1.375(5)
C(4)-C(5)	1.387(4)	C(5)-C(6)	1.397(4)
C(6)-C(7)	1.523(4)	C(7)-N(8)	1.250(3)
C(7)-N(9)	1.462(4)	N(9)-C(11)	1.450(4)
N(9)-C(10)	1.463(4)	C(11)-C(12)	1.514(4)
C(12)-N(13)	1.471(4)	N(13)-C(14)	1.464(4)
N(13)-C(15)	1.465(4)	C(16)-C(17)	1.379(5)
C(16)-C(21)	1.394(4)	C(17)-C(18)	1.380(6)
C(18)-C(19)	1.379(6)	C(19)-C(20)	1.393(5)
C(20)-C(21)	1.391(4)	C(21)-C(22)	1.511(4)
C(22)-N(23)	1.257(4)	C(22)-N(24)	1.432(4)
N(24)-C(26)	1.450(4)	N(24)-C(25)	1.453(4)
C(26)-C(27)	1.527(4)	C(27)-N(28)	1.476(4)
N(28)-C(29)	1.462(4)	N(28)-C(30)	1.468(4)
C(31)-C(32)	1.383(4)	C(31)-C(36)	1.393(4)
C(32)-C(33)	1.384(4)	C(33)-C(34)	1.374(4)
C(34)-C(35)	1.383(4)	C(35)-C(36)	1.396(4)
C(36)-C(37)	1.510(4)	C(37)-N(38)	1.258(3)
C(37)-N(39)	1.427(4)	N(39)-C(41)	1.451(4)
N(39)-C(40)	1.462(3)	C(41)-C(42)	1.514(4)
C(42)-N(43)	1.469(4)	N(43)-C(44)	1.460(4)
N(43)-C(45)	1.477(4)	C(46)-C(47)	1.384(4)
C(46)-C(51)	1.393(4)	C(47)-C(48)	1.374(4)
C(48)-C(49)	1.380(4)	C(49)-C(50)	1.387(4)
C(50)-C(51)	1.390(4)	C(51)-C(52)	1.520(4)
C(52)-N(53)	1.251(3)	C(52)-N(54)	1.445(3)
N(54)-C(55)	1.456(4)	N(54)-C(56)	1.463(4)
C(56)-C(57)	1.526(4)	C(57)-N(58)	1.472(4)
N(58)-C(59)	1.461(4)	N(58)-C(60)	1.463(4)

N(38)-Li(1)-N(53)	102.4(2)	N(38)-Li(1)-N(23)	98.7(2)
N(53)-Li(1)-N(23)	99.5(2)	N(38)-Li(1)-N(28)	121.3(2)
N(53)-Li(1)-N(28)	125.4(2)	N(23)-Li(1)-N(28)	103.9(2)
N(38)-Li(1)-Li(3)	50.1(2)	N(53)-Li(1)-Li(3)	52.9(2)
N(23)-Li(1)-Li(3)	98.2(2)	N(28)-Li(1)-Li(3)	157.5(2)
N(38)-Li(1)-Li(4)	50.9(2)	N(53)-Li(1)-Li(4)	98.7(2)
N(23)-Li(1)-Li(4)	48.8(2)	N(28)-Li(1)-Li(4)	133.4(2)
Li(3)-Li(1)-Li(4)	61.4(2)	N(38)-Li(1)-Li(2)	97.1(2)
N(53)-Li(1)-Li(2)	50.0(2)	N(23)-Li(1)-Li(2)	50.7(2)
N(28)-Li(1)-Li(2)	138.4(2)	Li(3)-Li(1)-Li(2)	61.1(2)
Li(4)-Li(1)-Li(2)	59.6(2)	N(8)-Li(2)-N(53)	100.4(2)
N(8)-Li(2)-N(23)	99.9(2)	N(53)-Li(2)-N(23)	98.7(2)
N(8)-Li(2)-N(58)	126.7(2)	N(53)-Li(2)-N(58)	108.1(2)
N(23)-Li(2)-N(58)	118.4(2)	N(8)-Li(2)-Li(4)	51.8(2)
N(53)-Li(2)-Li(4)	98.1(2)	N(23)-Li(2)-Li(4)	48.7(2)
N(58)-Li(2)-Li(4)	152.9(2)	N(8)-Li(2)-Li(1)	96.4(2)
N(53)-Li(2)-Li(1)	49.5(2)	N(23)-Li(2)-Li(1)	50.5(2)

N(58)-Li(2)-Li(1)	136.2(2)	Li(4)-Li(2)-Li(1)	59.4(2)
N(8)-Li(2)-Li(3)	50.0(2)	N(53)-Li(2)-Li(3)	51.5(2)
N(23)-Li(2)-Li(3)	95.8(2)	N(58)-Li(2)-Li(3)	143.9(2)
Li(4)-Li(2)-Li(3)	60.4(2)	Li(1)-Li(2)-Li(3)	58.3(2)
N(38)-Li(3)-N(8)	100.0(2)	N(38)-Li(3)-N(53)	100.0(2)
N(8)-Li(3)-N(53)	97.2(2)	N(38)-Li(3)-N(13)	134.6(2)
N(8)-Li(3)-N(13)	105.2(2)	N(53)-Li(3)-N(13)	113.2(2)
N(38)-Li(3)-Li(1)	50.3(2)	N(8)-Li(3)-Li(1)	97.4(2)
N(53)-Li(3)-Li(1)	50.2(2)	N(13)-Li(3)-Li(1)	154.1(2)
N(38)-Li(3)-Li(4)	50.1(2)	N(8)-Li(3)-Li(4)	50.9(2)
N(53)-Li(3)-Li(4)	95.4(2)	N(13)-Li(3)-Li(4)	146.1(2)
Li(1)-Li(3)-Li(4)	59.6(2)	N(38)-Li(3)-Li(2)	96.9(2)
N(8)-Li(3)-Li(2)	48.9(2)	N(53)-Li(3)-Li(2)	49.4(2)
N(13)-Li(3)-Li(2)	128.1(2)	Li(1)-Li(3)-Li(2)	60.6(2)
Li(4)-Li(3)-Li(2)	58.9(2)	N(23)-Li(4)-N(38)	100.6(2)
N(23)-Li(4)-N(8)	100.8(2)	N(38)-Li(4)-N(8)	97.7(2)
N(23)-Li(4)-N(43)	130.7(3)	N(38)-Li(4)-N(43)	102.7(2)
N(8)-Li(4)-N(43)	118.1(2)	N(23)-Li(4)-Li(1)	51.8(2)
N(38)-Li(4)-Li(1)	49.8(2)	N(8)-Li(4)-Li(1)	96.0(2)
N(43)-Li(4)-Li(1)	140.3(2)	N(23)-Li(4)-Li(2)	51.9(2)
N(38)-Li(4)-Li(2)	97.5(2)	N(8)-Li(4)-Li(2)	49.6(2)
N(43)-Li(4)-Li(2)	158.0(2)	Li(1)-Li(4)-Li(2)	61.0(2)
N(23)-Li(4)-Li(3)	98.5(2)	N(38)-Li(4)-Li(3)	48.8(2)
N(8)-Li(4)-Li(3)	49.9(2)	N(43)-Li(4)-Li(3)	129.2(2)
Li(1)-Li(4)-Li(3)	59.0(2)	Li(2)-Li(4)-Li(3)	60.7(2)
C(2)-C(1)-C(6)	121.3(3)	C(1)-C(2)-C(3)	120.0(3)
C(4)-C(3)-C(2)	119.2(3)	C(3)-C(4)-C(5)	120.7(3)
C(4)-C(5)-C(6)	120.6(3)	C(1)-C(6)-C(5)	118.2(3)
C(1)-C(6)-C(7)	119.0(2)	C(5)-C(6)-C(7)	122.6(3)
N(8)-C(7)-N(9)	124.4(2)	N(8)-C(7)-C(6)	123.6(2)
N(9)-C(7)-C(6)	111.7(2)	C(7)-N(8)-Li(2)	129.0(2)
C(7)-N(8)-Li(3)	140.6(2)	Li(2)-N(8)-Li(3)	81.1(2)
C(7)-N(8)-Li(4)	126.2(2)	Li(2)-N(8)-Li(4)	78.6(2)
Li(3)-N(8)-Li(4)	79.2(2)	C(11)-N(9)-C(7)	112.4(2)
C(11)-N(9)-C(10)	113.5(2)	C(7)-N(9)-C(10)	115.4(2)
N(9)-C(11)-C(12)	111.5(2)	N(13)-C(12)-C(11)	113.9(2)
C(14)-N(13)-C(15)	108.6(3)	C(14)-N(13)-C(12)	110.3(2)
C(15)-N(13)-C(12)	109.1(2)	C(14)-N(13)-Li(3)	119.1(2)
C(15)-N(13)-Li(3)	109.1(2)	C(12)-N(13)-Li(3)	100.2(2)
C(17)-C(16)-C(21)	121.1(3)	C(16)-C(17)-C(18)	120.2(3)
C(19)-C(18)-C(17)	119.8(3)	C(18)-C(19)-C(20)	120.2(4)
C(21)-C(20)-C(19)	120.5(3)	C(20)-C(21)-C(16)	118.2(3)
C(20)-C(21)-C(22)	121.1(3)	C(16)-C(21)-C(22)	120.3(3)
N(23)-C(22)-N(24)	124.9(2)	N(23)-C(22)-C(21)	121.4(2)
N(24)-C(22)-C(21)	113.5(2)	C(22)-N(23)-Li(4)	138.7(2)
C(22)-N(23)-Li(1)	123.7(2)	Li(4)-N(23)-Li(1)	79.4(2)
C(22)-N(23)-Li(2)	134.3(2)	Li(4)-N(23)-Li(2)	79.4(2)
Li(1)-N(23)-Li(2)	78.7(2)	C(22)-N(24)-C(26)	116.4(2)
C(22)-N(24)-C(25)	122.1(2)	C(26)-N(24)-C(25)	115.2(2)
N(24)-C(26)-C(27)	116.7(2)	N(28)-C(27)-C(26)	114.6(2)
C(29)-N(28)-C(30)	107.5(2)	C(29)-N(28)-C(27)	110.3(2)
C(30)-N(28)-C(27)	110.1(2)	C(29)-N(28)-Li(1)	112.5(2)
C(30)-N(28)-Li(1)	110.1(2)	C(27)-N(28)-Li(1)	106.4(2)
C(32)-C(31)-C(36)	121.2(3)	C(31)-C(32)-C(33)	120.0(3)
C(34)-C(33)-C(32)	119.6(3)	C(33)-C(34)-C(35)	120.5(3)
C(34)-C(35)-C(36)	121.0(3)	C(31)-C(36)-C(35)	117.6(3)
C(31)-C(36)-C(37)	121.5(2)	C(35)-C(36)-C(37)	120.4(2)
N(38)-C(37)-N(39)	124.5(2)	N(38)-C(37)-C(36)	121.1(2)
N(39)-C(37)-C(36)	114.0(2)	C(37)-N(38)-Li(3)	134.9(2)
C(37)-N(38)-Li(1)	134.0(2)	Li(3)-N(38)-Li(1)	79.6(2)
C(37)-N(38)-Li(4)	127.0(2)	Li(3)-N(38)-Li(4)	81.2(2)
Li(1)-N(38)-Li(4)	79.3(2)	C(37)-N(39)-C(41)	116.8(2)
C(37)-N(39)-C(40)	121.0(2)	C(41)-N(39)-C(40)	114.7(2)

N(39)-C(41)-C(42)	116.8(2)	N(43)-C(42)-C(41)	114.5(2)
C(44)-N(43)-C(42)	109.9(3)	C(44)-N(43)-C(45)	108.8(2)
C(42)-N(43)-C(45)	110.4(2)	C(44)-N(43)-Li(4)	112.3(2)
C(42)-N(43)-Li(4)	109.2(2)	C(45)-N(43)-Li(4)	106.2(2)
C(47)-C(46)-C(51)	121.5(3)	C(48)-C(47)-C(46)	120.3(2)
C(47)-C(48)-C(49)	119.2(2)	C(48)-C(49)-C(50)	120.5(3)
C(49)-C(50)-C(51)	121.0(2)	C(50)-C(51)-C(46)	117.4(2)
C(50)-C(51)-C(52)	120.2(2)	C(46)-C(51)-C(52)	122.1(2)
N(53)-C(52)-N(54)	124.3(2)	N(53)-C(52)-C(51)	123.1(2)
N(54)-C(52)-C(51)	112.4(2)	C(52)-N(53)-Li(1)	129.3(2)
C(52)-N(53)-Li(2)	140.1(2)	Li(1)-N(53)-Li(2)	80.5(2)
C(52)-N(53)-Li(3)	128.1(2)	Li(1)-N(53)-Li(3)	76.9(2)
Li(2)-N(53)-Li(3)	79.1(2)	C(52)-N(54)-C(55)	120.3(2)
C(52)-N(54)-C(56)	112.7(2)	C(55)-N(54)-C(56)	114.2(2)
N(54)-C(56)-C(57)	111.9(2)	N(58)-C(57)-C(56)	113.1(2)
C(59)-N(58)-C(60)	108.7(2)	C(59)-N(58)-C(57)	110.5(2)
C(60)-N(58)-C(57)	109.3(2)	C(59)-N(58)-Li(2)	119.6(2)
C(60)-N(58)-Li(2)	109.0(2)	C(57)-N(58)-Li(2)	99.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

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

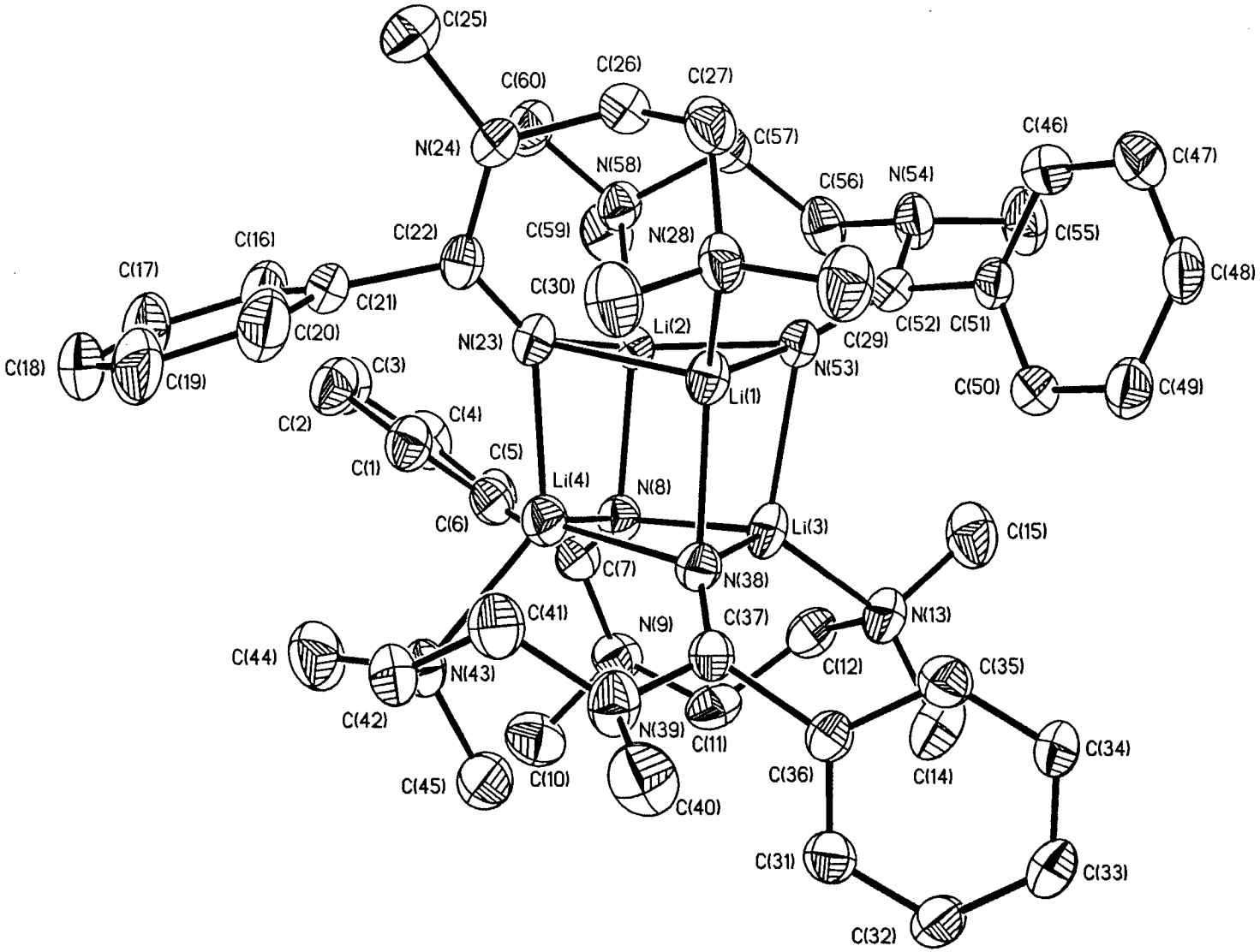
	U11	U22	U33	U23	U13	U12
Li(1)	20(2)	26(2)	26(2)	1(2)	7(2)	8(2)
Li(2)	29(2)	25(2)	26(2)	3(2)	7(2)	12(2)
Li(3)	21(2)	27(2)	28(2)	-5(2)	7(2)	4(2)
Li(4)	32(2)	27(2)	29(2)	4(2)	11(2)	13(2)
C(1)	34(2)	41(2)	36(2)	4(1)	12(1)	15(1)
C(2)	46(2)	44(2)	36(2)	-3(1)	13(1)	13(2)
C(3)	57(2)	50(2)	33(2)	3(1)	20(1)	27(2)
C(4)	42(2)	58(2)	38(2)	10(1)	22(1)	25(2)
C(5)	35(2)	44(2)	34(1)	9(1)	15(1)	16(1)
C(6)	33(2)	31(1)	28(1)	9(1)	12(1)	14(1)
C(7)	23(1)	26(1)	33(1)	1(1)	7(1)	9(1)
N(8)	26(1)	28(1)	29(1)	5(1)	11(1)	11(1)
N(9)	38(1)	26(1)	36(1)	7(1)	16(1)	9(1)
C(10)	44(2)	40(2)	52(2)	21(1)	24(2)	18(1)
C(11)	34(2)	22(1)	50(2)	2(1)	17(1)	8(1)
C(12)	23(1)	30(1)	47(2)	-7(1)	10(1)	4(1)
N(13)	24(1)	33(1)	35(1)	-3(1)	6(1)	8(1)
C(14)	49(2)	47(2)	49(2)	-13(2)	12(2)	16(2)
C(15)	29(2)	48(2)	46(2)	3(1)	0(1)	7(1)
C(16)	46(2)	41(2)	30(2)	-3(1)	4(1)	9(1)
C(17)	77(3)	56(2)	28(2)	-2(1)	2(2)	15(2)
C(18)	96(3)	50(2)	35(2)	-2(2)	-21(2)	24(2)
C(19)	60(2)	59(2)	62(2)	-11(2)	-24(2)	29(2)
C(20)	42(2)	53(2)	42(2)	-9(1)	-6(1)	18(2)
C(21)	30(2)	24(1)	31(1)	-3(1)	0(1)	6(1)
C(22)	21(1)	26(1)	26(1)	-1(1)	6(1)	10(1)
N(23)	23(1)	26(1)	25(1)	-1(1)	5(1)	10(1)
N(24)	33(1)	23(1)	31(1)	-1(1)	4(1)	9(1)
C(25)	41(2)	27(1)	49(2)	-2(1)	0(1)	5(1)
C(26)	33(2)	25(1)	35(1)	4(1)	6(1)	14(1)
C(27)	32(2)	31(1)	34(1)	10(1)	10(1)	8(1)
N(28)	27(1)	33(1)	27(1)	5(1)	9(1)	12(1)
C(29)	40(2)	44(2)	36(2)	2(1)	14(1)	12(1)
C(30)	35(2)	49(2)	37(2)	6(1)	13(1)	20(1)
C(31)	56(2)	31(1)	28(1)	7(1)	17(1)	25(1)
C(32)	58(2)	27(1)	35(2)	2(1)	18(1)	20(1)
C(33)	51(2)	35(2)	33(2)	-6(1)	10(1)	24(1)
C(34)	52(2)	36(2)	28(1)	5(1)	12(1)	25(1)
C(35)	36(2)	30(1)	34(1)	5(1)	13(1)	20(1)
C(36)	31(1)	28(1)	31(1)	4(1)	13(1)	19(1)
C(37)	27(1)	27(1)	26(1)	7(1)	11(1)	14(1)
N(38)	24(1)	26(1)	28(1)	3(1)	9(1)	12(1)
N(39)	27(1)	45(1)	33(1)	-1(1)	10(1)	21(1)
C(40)	39(2)	58(2)	51(2)	8(2)	18(1)	33(2)
C(41)	22(1)	41(2)	42(2)	4(1)	4(1)	13(1)
C(42)	37(2)	37(2)	34(2)	2(1)	-3(1)	18(1)
N(43)	39(1)	35(1)	26(1)	5(1)	8(1)	18(1)
C(44)	72(2)	57(2)	34(2)	6(1)	13(2)	34(2)
C(45)	48(2)	34(2)	41(2)	8(1)	14(1)	15(1)
C(46)	53(2)	26(1)	30(1)	4(1)	10(1)	20(1)
C(47)	48(2)	33(2)	29(1)	9(1)	11(1)	14(1)
C(48)	32(2)	41(2)	21(1)	2(1)	7(1)	11(1)

C(49)	34(2)	33(1)	32(1)	0(1)	9(1)	18(1)
C(50)	30(1)	26(1)	31(1)	6(1)	8(1)	13(1)
C(51)	26(1)	28(1)	21(1)	1(1)	1(1)	11(1)
C(52)	25(1)	20(1)	27(1)	-1(1)	5(1)	8(1)
N(53)	22(1)	24(1)	26(1)	1(1)	5(1)	9(1)
N(54)	36(1)	42(1)	26(1)	1(1)	4(1)	24(1)
C(55)	45(2)	63(2)	34(2)	0(1)	-2(1)	34(2)
C(56)	31(2)	48(2)	34(1)	4(1)	8(1)	25(1)
C(57)	37(2)	31(1)	32(1)	7(1)	13(1)	21(1)
N(58)	33(1)	31(1)	27(1)	3(1)	11(1)	15(1)
C(59)	44(2)	49(2)	41(2)	9(1)	21(1)	23(2)
C(60)	44(2)	38(2)	37(2)	-5(1)	8(1)	19(1)

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

	x	y	z	U(eq)
H(1A)	8253(3)	1823(3)	4056(1)	43
H(2A)	8123(3)	3011(3)	4881(1)	52
H(3A)	6078(3)	2619(3)	5138(1)	52
H(4A)	4209(3)	979(3)	4586(1)	51
H(5A)	4354(3)	-278(3)	3790(1)	44
H(10A)	5752(22)	-1690(8)	4082(2)	65
H(10B)	6410(13)	-2413(18)	3725(6)	65
H(10C)	4868(10)	-2973(10)	3661(5)	65
H(11A)	5041(3)	-2993(2)	2601(1)	42
H(11B)	6404(3)	-1896(2)	2557(1)	42
H(12A)	3943(3)	-2232(3)	1909(1)	42
H(12B)	4729(3)	-799(3)	2202(1)	42
H(14A)	4654(3)	-3075(9)	1117(10)	73
H(14B)	5989(20)	-2853(12)	1573(3)	73
H(14C)	6008(20)	-2265(5)	933(7)	73
H(15A)	3954(7)	-1326(9)	930(7)	66
H(15B)	5300(13)	-530(20)	736(5)	66
H(15C)	4841(19)	70(11)	1249(3)	66
H(16A)	10044(3)	4107(3)	4307(1)	50
H(17A)	11061(4)	3973(3)	5292(1)	69
H(18A)	13130(5)	3876(3)	5473(2)	80
H(19A)	14170(4)	3888(4)	4659(2)	77
H(20A)	13173(3)	4068(3)	3668(2)	57
H(25A)	12366(18)	6338(3)	3677(4)	64
H(25B)	11356(5)	6853(9)	3296(9)	64
H(25C)	12639(14)	6974(8)	3062(6)	64
H(26A)	10477(3)	6024(3)	2275(1)	37
H(26B)	9663(3)	4530(3)	2256(1)	37
H(27A)	10635(3)	5045(3)	1392(1)	39
H(27B)	12043(3)	5621(3)	1820(1)	39
H(29A)	10502(10)	3285(20)	831(2)	61
H(29B)	11330(21)	2465(9)	1084(2)	61
H(29C)	12053(12)	3937(12)	987(4)	61
H(30A)	13223(3)	4350(14)	2010(6)	58
H(30B)	12526(10)	2874(6)	2105(7)	58
H(30C)	12475(9)	3939(19)	2556(2)	58
H(31A)	8872(3)	-2864(3)	1988(1)	41
H(32A)	7676(3)	-4392(3)	1168(1)	46
H(33A)	7461(3)	-3761(3)	173(1)	45
H(34A)	8395(3)	-1593(3)	11(1)	42
H(35A)	9562(3)	-54(3)	829(1)	37
H(40A)	12518(16)	-972(20)	2464(2)	66
H(40B)	12605(14)	51(6)	1975(9)	66
H(40C)	11513(3)	-1360(14)	1830(7)	66
H(41A)	11464(3)	1449(3)	2842(1)	42
H(41B)	12698(3)	1072(3)	2946(1)	42
H(42A)	11751(3)	-414(3)	3640(1)	44
H(42B)	12076(3)	1030(3)	3866(1)	44
H(44A)	10500(22)	-321(19)	4522(2)	77
H(44B)	9195(4)	-72(22)	4322(2)	77
H(44C)	10575(21)	1091(5)	4412(3)	77
H(45A)	9384(17)	-1582(5)	3002(3)	61
H(45B)	8434(5)	-1627(5)	3452(9)	61

H(45C)	9687(13)	-1950(3)	3679(6)	61
H(46A)	7739(3)	4228(3)	436(1)	42
H(47A)	8717(3)	4286(3)	-399(1)	44
H(48A)	9077(3)	2498(3)	-721(1)	39
H(49A)	8496(3)	665(3)	-182(1)	37
H(50A)	7602(3)	632(2)	681(1)	34
H(55A)	5344(6)	2439(21)	307(2)	68
H(55B)	4678(15)	3252(10)	596(6)	68
H(55C)	4298(10)	1782(12)	714(4)	68
H(56A)	5510(3)	2163(3)	1974(1)	41
H(56B)	4751(3)	3030(3)	1699(1)	41
H(57A)	7405(3)	4483(2)	2091(1)	36
H(57B)	6219(3)	4779(2)	2242(1)	36
H(59A)	5318(12)	3976(8)	3119(9)	62
H(59B)	5863(5)	3099(20)	3541(3)	62
H(59C)	5005(8)	2540(12)	2881(6)	62
H(60A)	7534(9)	5565(7)	3260(8)	58
H(60B)	8656(7)	5174(12)	3097(5)	58
H(60C)	8039(15)	4646(6)	3670(2)	58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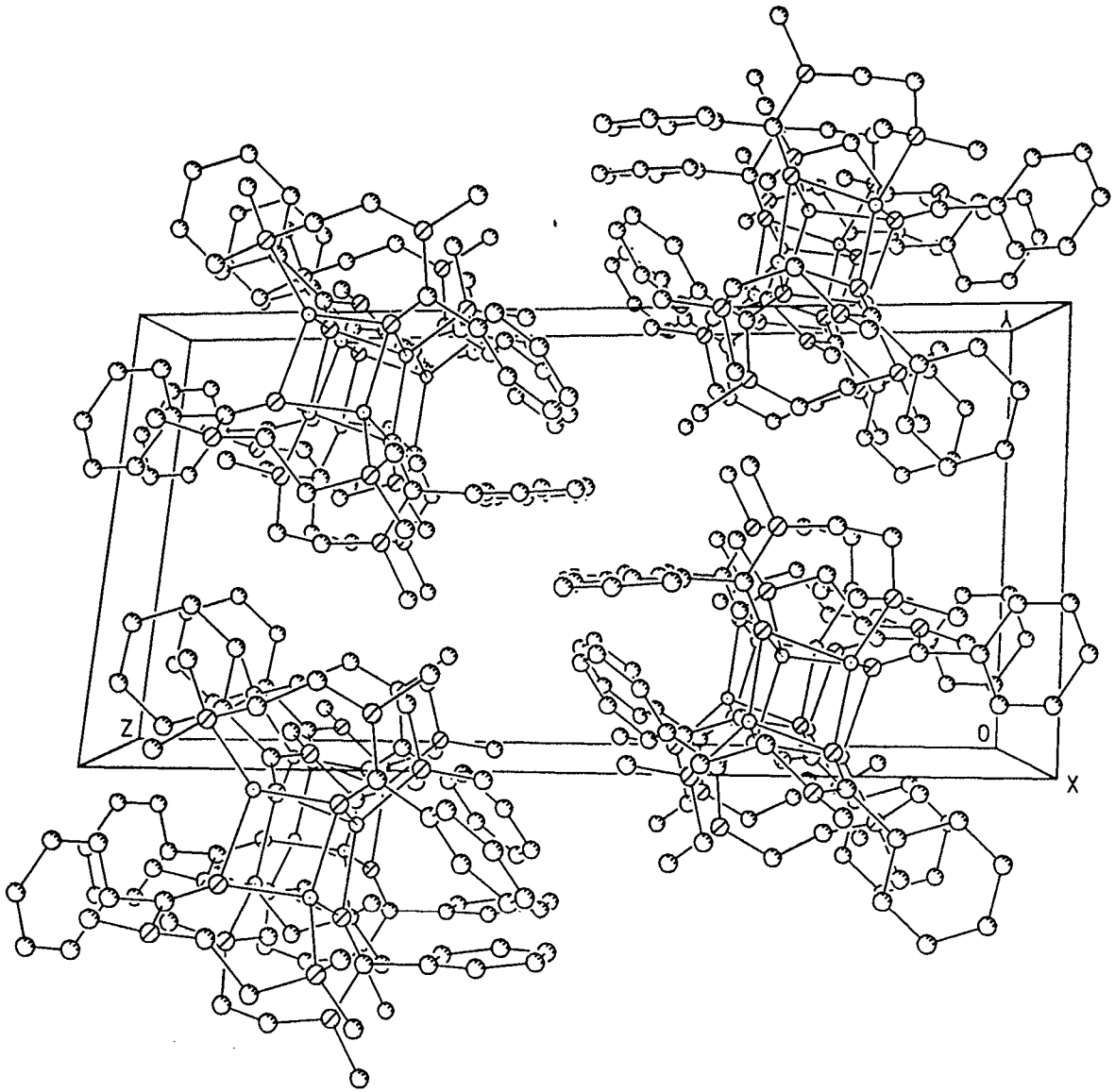
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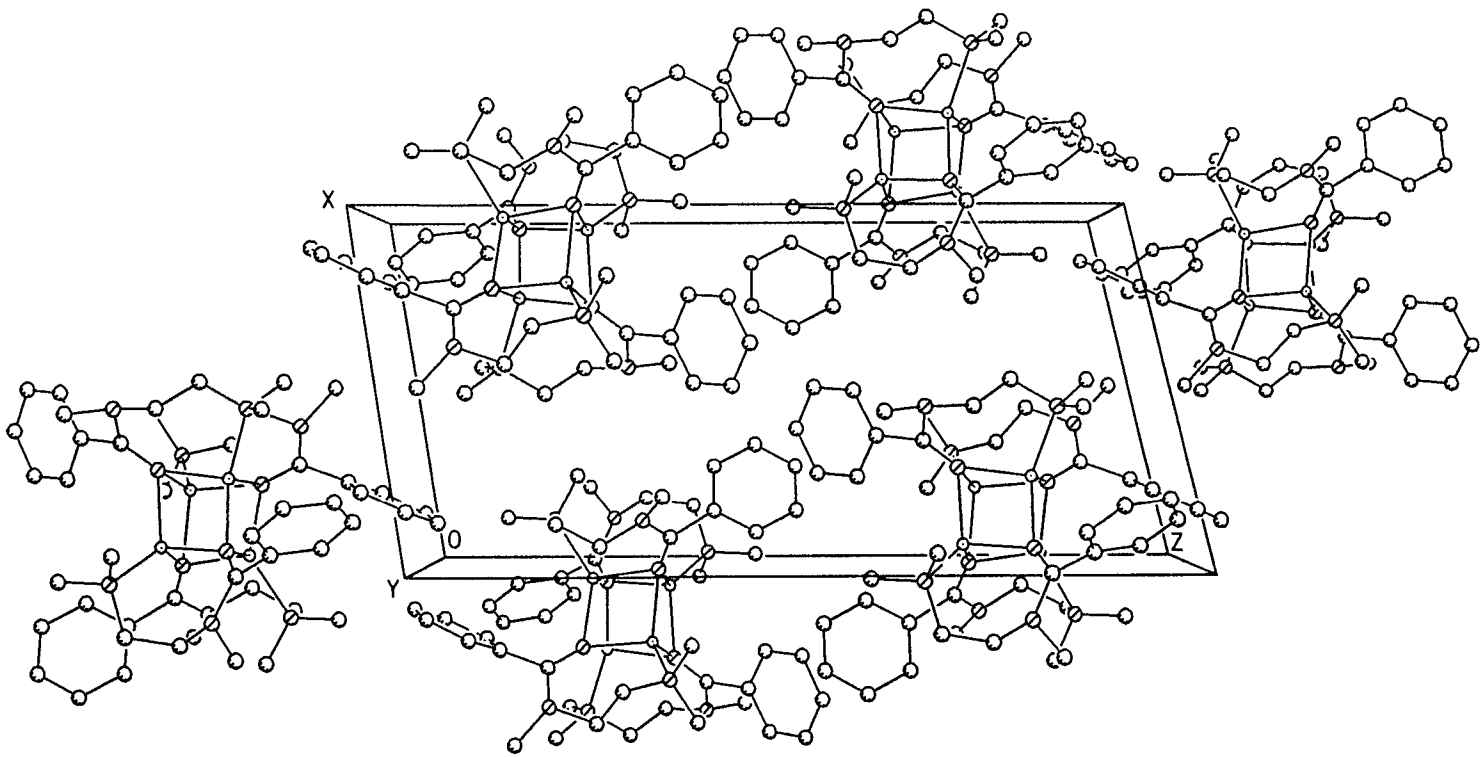
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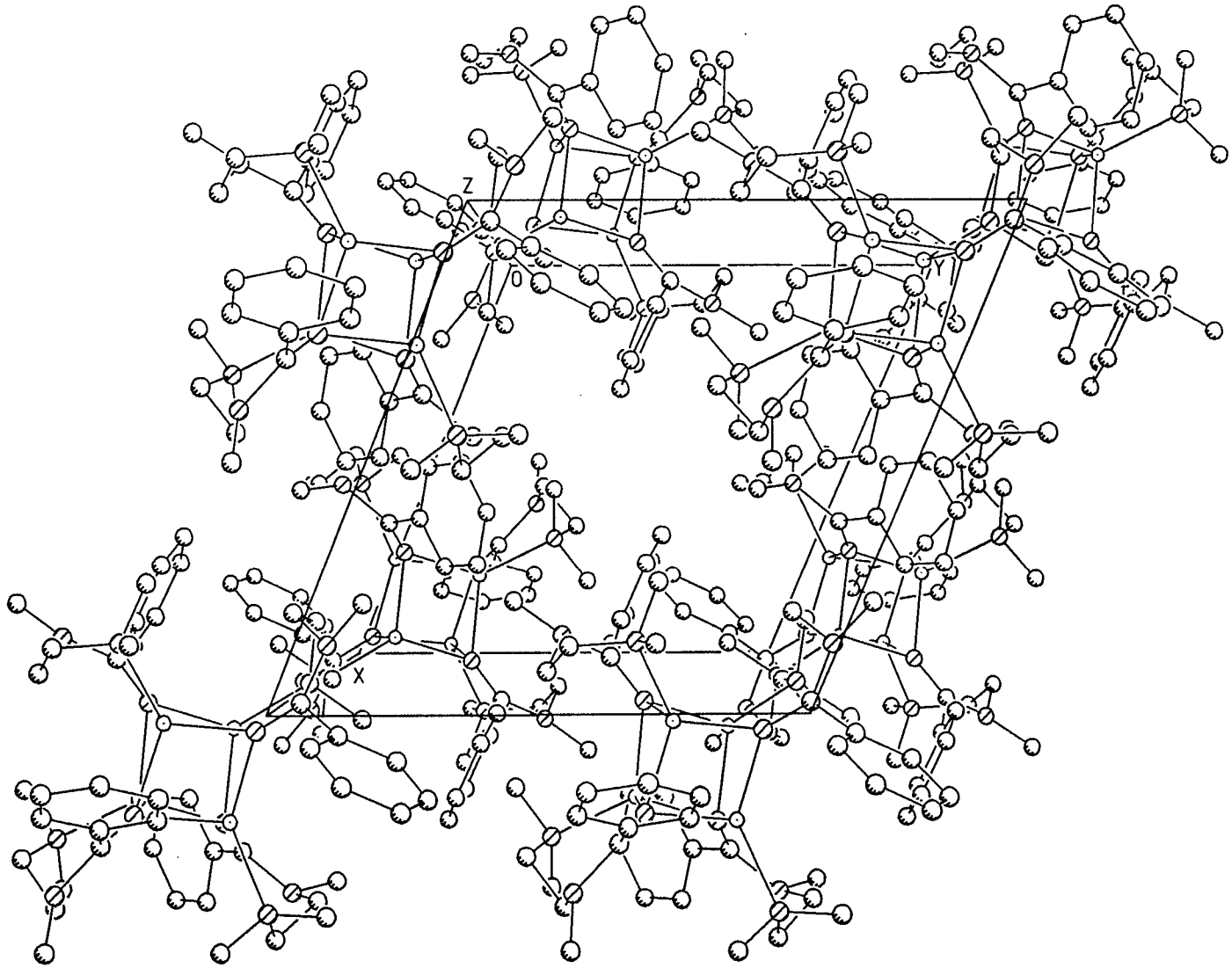
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