Table 1. Crystal data and structure refinement for LZU1.

Identification code	ABClzu1 (12/8-2000)
Empirical formula	$C_{25}H_{23}NO$
Formula weight	353.44
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 14.494(3) Å alpha = 90° b = 17.802(3) Å beta = 113.136(4)° c = 16.530(3) Å gamma = 90°
Volume, Z	3922.1(12) $Å^3$, 8
Density (calculated)	1.197 Mg/m^3
Absorption coefficient	0.072 mm^{-1}
F(000)	1504
Crystal size	0.30 x 0.22 x 0.20 mm
θ range for data collection	1.59 to 27.58°
Limiting indices	$-15 \le h \le 18$, $-23 \le k \le 23$, $-21 \le l \le 21$
Reflections collected	26195
Independent reflections	9055 (R_{int} = 0.0542)
Completeness to θ = 27.58°	99.7 %
Absorption correction	SADABS
Max. and min. transmission	0.9857 and 0.9787
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9055 / 0 / 604
Goodness-of-fit on F^2	0.741
Final R indices [I>2σ(I)]	R1 = 0.0506, wR2 = 0.1323
R indices (all data)	R1 = 0.1613, wR2 = 0.1798
Extinction coefficient	0.0000(2)
Largest diff. peak and hole	0.348 and -0.231 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for LZU1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	7419(1)	2056(1)	3651(1)	75(1)
N(1)	9030(1)	2213(1)	5008(1)	58(1)
C(1)	10978(1)	1702(1)	6498(1)	63(1)
C(2)	11678(2)	1422(1)	7274(2)	79(1)
C(3)	11691(2)	673(2)	7481(2)	81(1)
C(4)	10984(2)	209(1)	6911(2)	78(1)
C(5)	10278(2)	485(1)	6135(1)	63(1)
C(6)	10265(1)	1235(1)	5911(1)	50(1)
C(7)	9544(1)	1504(1)	5019(1)	52(1)
C(8)	10066(2)	1592(1)	4384(1)	62(1)
C(9)	8426(1)	2243(1)	5552(1)	49(1)
C(10)	8294(1)	3068(1)	5734(1)	52(1)
C(11)	8748(2)	3359(1)	6553(2)	86(1)
C(12)	8676(2)	4122(1)	6713(2)	104(1)
C(13)	8148(2)	4589(1)	6047(2)	82(1)
C(14)	7677(2)	4303(1)	5222(2)	77(1)
C(15)	7748(2)	3548(1)	5069(1)	65(1)
C(16)	7431(1)	1840(1)	5093(1)	47(1)
C(17)	6992(1)	1772(1)	4186(1)	56(1)
C(18)	6063(2)	1405(1)	3769(1)	67(1)
C(19)	5560(2)	1123(1)	4234(2)	68(1)
C(20)	5960(1)	1181(1)	5155(1)	57(1)
C(21)	5447(2)	876(1)	5651(2)	71(1)
C(22)	5849(2)	904(1)	6538(2)	79(1)
C(23)	6775(2)	1241(1)	6973(1)	76(1)
C(24)	7289(2)	1555(1)	6517(1)	61(1)
C(25)	6914(1)	1533(1)	5594(1)	48(1)
O(2)	13651(1)	3037(1)	7012(1)	87(1)
N(2)	14284(1)	2749(1)	5781(1)	65(1)
C(26)	14251(2)	4268(1)	4397(2)	85(1)
C(27)	14193(2)	4430(1)	3562(2)	107(1)
C(28)	14634(2)	3967(2)	3160(2)	94(1)
C(29)	15093(2)	3338(2)	3576(2)	96(1)
C(30)	15145(2)	3171(1)	4395(2)	81(1)
C(31)	14730(1)	3635(1)	4830(1)	61(1)
C(32)	14795(2)	3452(1)	5739(2)	66(1)
C(33)	15872(2)	3396(2)	6409(2)	86(1)
C(34)	13222(1)	2693(1)	5169(1)	55(1)
C(35)	12946(1)	1872(1)	5003(2)	63(1)
C(36)	12875(2)	1430(1)	5662(2)	83(1)
C(37)	12652(2)	672(1)	5521(2)	114(1)
C(38)	12491(2)	362(2)	4721(3)	132(1)
C(39)	12563(2)	786(2)	4065(2)	119(1)
C(40)	12795(2)	1547(2)	4207(2)	87(1)
C(41)	12537(1)	3134(1)	5491(1)	51(1)
C(42)	12780(2)	3277(1)	6370(1)	63(1)
C(43)	12135(2)	3678(1)	6678(2)	76(1)
C(44)	11246(2)	3924(1)	6078(2)	78(1)

C(45)	10928(2)	3788(1)	5165(2)	63(1)
C(46)	9983(2)	4020(1)	4552(2)	85(1)
C(47)	9687(2)	3865(2)	3682(2)	98(1)
C(48)	10313(2)	3466(1)	3384(2)	81(1)
C(49)	11239(2)	3238(1)	3958(1)	61(1)
C(50)	11587(1)	3387(1)	4866(1)	52(1)

Table 3. Bond lengths [Å] and angles [°] for LZU1.

O(1)-C(17)	1.361(2)	N(1)-C(7)	1.463(2)
N(1)-C(9)	1.483(2)	C(1)-C(2)	1.379(3)
C(1)-C(6)	1.384(2)	C(2)-C(3)	1.375(3)
C(3)-C(4)	1.365(3)	C(4)-C(5)	1.380(3)
C(5)-C(6)	1.384(3)	C(6)-C(7)	1.510(2)
C(7)-C(8)	1.525(3)	C(9)-C(16)	1.520(2)
C(9)-C(10)	1.526(3)	C(10)-C(11)	1.354(3)
C(10)-C(15)	1.371(3)	C(11)-C(12)	1.395(3)
C(12)-C(13)	1.352(3)	C(13)-C(14)	1.360(3)
C(14)-C(15)	1.378(3)	C(16)-C(17)	1.384(3)
C(16)-C(25)	1.425(3)	C(17)-C(18)	1.408(3)
C(18)-C(19)	1.348(3)	C(19)-C(20)	1.403(3)
C(20)-C(21)	1.414(3)	C(20)-C(25)	1.430(2)
C(21)-C(22)	1.349(3)	C(22)-C(23)	1.385(3)
C(23)-C(24)	1.371(3)	C(24)-C(25)	1.405(3)
O(2)-C(42)	1.360(2)	N(2)-C(32)	1.470(3)
N(2)-C(34)	1.476(2)	C(26)-C(31)	1.370(3)
C(26)-C(27)	1.380(4)	C(27)-C(28)	1.365(4)
C(28)-C(29)	1.345(3)	C(29)-C(30)	1.359(3)
C(30)-C(31)	1.379(3)	C(31)-C(32)	1.503(3)
C(32)-C(33)	1.522(3)	C(34)-C(35)	1.512(3)
C(34)-C(41)	1.516(3)	C(35)-C(40)	1.374(3)
C(35)-C(36)	1.381(3)	C(36)-C(37)	1.385(3)
C(37)-C(38)	1.365(4)	C(38)-C(39)	1.359(4)
C(39)-C(40)	1.392(4)	C(41)-C(42)	1.378(3)
C(41)-C(50)	1.430(2)	C(42)-C(43)	1.420(3)
C(43)-C(44)	1.353(3)	C(44)-C(45)	1.416(3)
C(45)-C(46)	1.407(3)	C(45)-C(50)	1.426(3)
C(46)-C(47)	1.358(4)	C(47)-C(48)	1.387(4)
C(48)-C(49)	1.365(3)	C(49)-C(50)	1.408(3)

C(7)-N(1)-C(9)	116.29(14)	C(2)-C(1)-C(6)	120.6(2)
C(3)-C(2)-C(1)	121.1(2)	C(4)-C(3)-C(2)	118.8(2)
C(3)-C(4)-C(5)	120.5(2)	C(4)-C(5)-C(6)	121.34(19)
C(1)-C(6)-C(5)	117.63(18)	C(1)-C(6)-C(7)	122.29(17)
C(5)-C(6)-C(7)	119.88(16)	N(1)-C(7)-C(6)	116.03(15)
N(1)-C(7)-C(8)	106.90(15)	C(6)-C(7)-C(8)	111.41(15)
N(1)-C(9)-C(16)	110.54(15)	N(1)-C(9)-C(10)	107.67(15)
C(16)-C(9)-C(10)	112.64(14)	C(11)-C(10)-C(15)	117.69(19)
C(11)-C(10)-C(9)	120.98(17)	C(15)-C(10)-C(9)	121.27(17)
C(10)-C(11)-C(12)	121.2(2)	C(13)-C(12)-C(11)	120.4(2)
C(12)-C(13)-C(14)	119.0(2)	C(13)-C(14)-C(15)	120.4(2)
C(10)-C(15)-C(14)	121.3(2)	C(17)-C(16)-C(25)	118.21(16)
C(17)-C(16)-C(9)	121.59(17)	C(25)-C(16)-C(9)	120.19(16)
O(1)-C(17)-C(16)	122.62(17)	O(1)-C(17)-C(18)	116.39(18)
C(16)-C(17)-C(18)	120.99(19)	C(19)-C(18)-C(17)	121.4(2)
C(18)-C(19)-C(20)	120.37(19)	C(19)-C(20)-C(21)	120.89(19)
C(19)-C(20)-C(25)	119.22(19)	C(21)-C(20)-C(25)	119.87(19)
C(22)-C(21)-C(20)	121.0(2)	C(21)-C(22)-C(23)	119.9(2)
C(24)-C(23)-C(22)	121.0(2)	C(23)-C(24)-C(25)	121.65(19)
C(24)-C(25)-C(16)	123.57(17)	C(24)-C(25)-C(20)	116.60(18)
C(16)-C(25)-C(20)	119.82(17)	C(32)-N(2)-C(34)	115.72(15)
C(31)-C(26)-C(27)	120.9(2)	C(28)-C(27)-C(26)	120.3(2)
C(29)-C(28)-C(27)	119.0(3)	C(28)-C(29)-C(30)	121.0(3)
C(29)-C(30)-C(31)	121.6(2)	C(26)-C(31)-C(30)	117.1(2)

C(26)-C(31)-C(32)	121.3(2)	C(30)-C(31)-C(32)	121.56(19)
N(2)-C(32)-C(31)	113.34(17)	N(2)-C(32)-C(33)	107.53(18)
C(31)-C(32)-C(33)	112.6(2)	N(2)-C(34)-C(35)	108.65(15)
N(2)-C(34)-C(41)	112.06(16)	C(35)-C(34)-C(41)	113.69(16)
C(40)-C(35)-C(36)	118.8(2)	C(40)-C(35)-C(34)	120.9(2)
C(36)-C(35)-C(34)	120.3(2)	C(35)-C(36)-C(37)	120.5(3)
C(38)-C(37)-C(36)	119.8(3)	C(39)-C(38)-C(37)	120.6(3)
C(38)-C(39)-C(40)	119.7(3)	C(35)-C(40)-C(39)	120.6(3)
C(42)-C(41)-C(50)	118.53(18)	C(42)-C(41)-C(34)	122.25(17)
C(50)-C(41)-C(34)	119.18(17)	O(2)-C(42)-C(41)	122.64(19)
O(2)-C(42)-C(43)	114.74(19)	C(41)-C(42)-C(43)	122.62(19)
C(44)-C(43)-C(42)	118.2(2)	C(43)-C(44)-C(45)	122.9(2)
C(46)-C(45)-C(44)	122.3(2)	C(46)-C(45)-C(50)	119.5(2)
C(44)-C(45)-C(50)	118.20(18)	C(47)-C(46)-C(45)	121.1(2)
C(46)-C(47)-C(48)	120.1(2)	C(49)-C(48)-C(47)	120.5(3)
C(48)-C(49)-C(50)	121.8(2)	C(49)-C(50)-C(45)	117.04(18)
C(49)-C(50)-C(41)	123.34(18)	C(45)-C(50)-C(41)	119.57(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for LZU1.

The anisotropic displacement factor exponent takes the form:

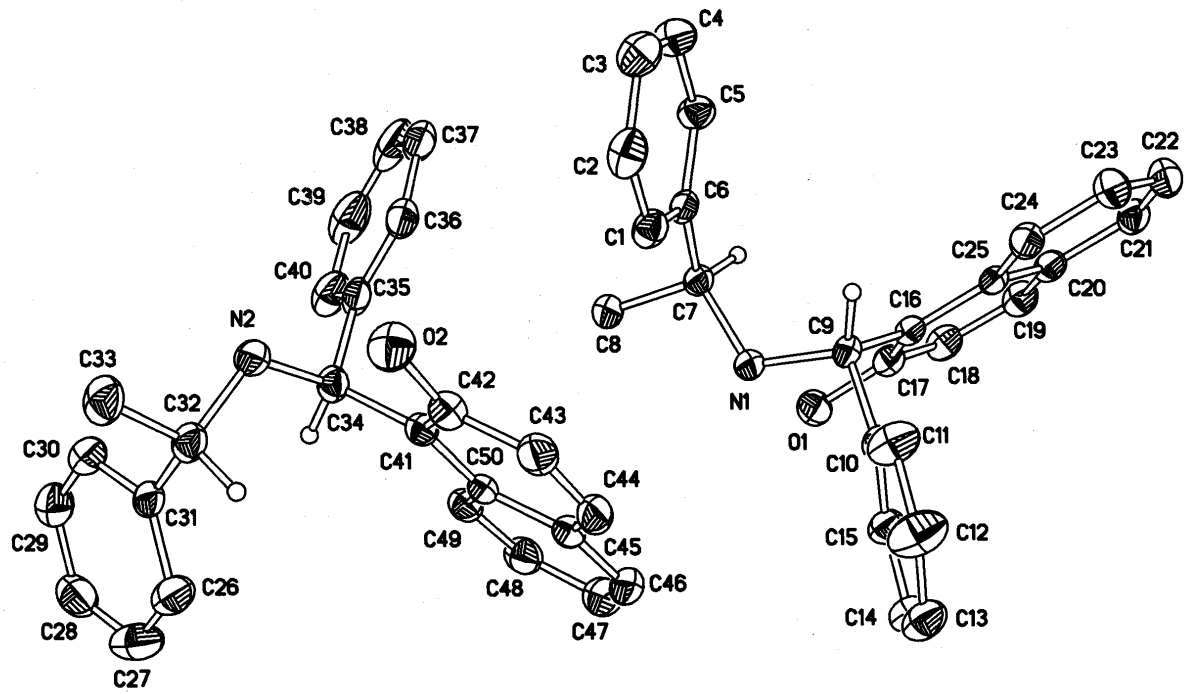
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
O(1)	80(1)	88(1)	64(1)	20(1)	36(1)	13(1)
N(1)	55(1)	41(1)	88(1)	4(1)	39(1)	3(1)
C(1)	51(1)	54(1)	83(1)	-12(1)	25(1)	-2(1)
C(2)	57(1)	91(2)	82(2)	-30(1)	20(1)	-8(1)
C(3)	70(2)	91(2)	68(2)	-3(1)	11(1)	10(1)
C(4)	77(2)	66(2)	81(2)	5(1)	23(1)	7(1)
C(5)	57(1)	52(1)	71(1)	-4(1)	17(1)	-2(1)
C(6)	41(1)	46(1)	66(1)	-4(1)	24(1)	3(1)
C(7)	43(1)	43(1)	70(1)	-3(1)	23(1)	-2(1)
C(8)	62(1)	57(1)	77(1)	2(1)	38(1)	5(1)
C(9)	38(1)	53(1)	57(1)	3(1)	20(1)	7(1)
C(10)	38(1)	53(1)	64(1)	-2(1)	17(1)	3(1)
C(11)	68(2)	73(2)	86(2)	-14(1)	-5(1)	6(1)
C(12)	98(2)	72(2)	102(2)	-33(2)	-1(2)	2(2)
C(13)	69(1)	58(1)	111(2)	-13(1)	25(1)	6(1)
C(14)	84(2)	58(1)	94(2)	5(1)	42(1)	17(1)
C(15)	73(1)	57(1)	68(1)	-3(1)	29(1)	11(1)
C(16)	43(1)	42(1)	54(1)	-2(1)	17(1)	6(1)
C(17)	49(1)	57(1)	58(1)	3(1)	17(1)	8(1)
C(18)	55(1)	73(1)	58(1)	-7(1)	7(1)	7(1)
C(19)	47(1)	65(1)	80(2)	-9(1)	13(1)	-4(1)
C(20)	48(1)	46(1)	74(1)	-4(1)	22(1)	3(1)
C(21)	56(1)	54(1)	110(2)	-2(1)	42(1)	-2(1)
C(22)	86(1)	69(1)	103(2)	5(1)	59(1)	0(1)
C(23)	87(1)	82(2)	70(1)	8(1)	43(1)	7(1)
C(24)	54(1)	68(1)	61(1)	-1(1)	22(1)	5(1)
C(25)	43(1)	43(1)	59(1)	4(1)	21(1)	9(1)
O(2)	77(1)	110(1)	59(1)	7(1)	12(1)	7(1)
N(2)	44(1)	64(1)	77(1)	13(1)	12(1)	2(1)
C(26)	72(2)	65(1)	105(2)	-6(1)	19(1)	10(1)
C(27)	114(2)	70(2)	109(2)	15(2)	13(2)	12(2)
C(28)	83(2)	96(2)	95(2)	16(2)	27(1)	-18(2)
C(29)	90(2)	102(2)	110(2)	15(2)	54(1)	12(2)
C(30)	74(1)	76(2)	102(2)	17(1)	44(1)	21(1)
C(31)	40(1)	55(1)	85(2)	0(1)	20(1)	-3(1)
C(32)	46(1)	58(1)	88(2)	-12(1)	20(1)	-2(1)
C(33)	53(1)	91(2)	100(2)	-10(2)	15(1)	-12(1)
C(34)	43(1)	62(1)	59(1)	-1(1)	18(1)	-3(1)
C(35)	40(1)	58(1)	93(2)	-12(1)	30(1)	0(1)
C(36)	61(1)	64(1)	136(2)	2(1)	52(1)	5(1)
C(37)	71(1)	62(2)	229(3)	17(2)	81(2)	10(1)
C(38)	61(2)	69(2)	263(4)	-48(2)	59(2)	5(1)
C(39)	74(2)	104(2)	169(3)	-57(2)	35(2)	4(2)
C(40)	65(1)	79(2)	111(2)	-28(2)	28(1)	3(1)
C(41)	53(1)	46(1)	57(1)	0(1)	25(1)	-3(1)
C(42)	64(1)	62(1)	63(1)	0(1)	26(1)	-4(1)
C(43)	83(1)	63(1)	94(2)	-7(1)	47(1)	-4(1)
C(44)	91(1)	54(1)	117(2)	-11(1)	73(1)	-3(1)

C(45)	56(1)	45(1)	94(2)	5(1)	37(1)	-1(1)
C(46)	58(1)	68(2)	138(2)	15(1)	47(1)	8(1)
C(47)	50(1)	92(2)	135(2)	35(2)	19(2)	3(1)
C(48)	60(1)	81(2)	87(2)	18(1)	15(1)	-8(1)
C(49)	53(1)	59(1)	68(1)	11(1)	20(1)	-4(1)
C(50)	48(1)	39(1)	71(1)	5(1)	26(1)	-5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for LZU1.

	x	y	z	U(eq)
H(1N)	9446(14)	2573(10)	5163(12)	75(6)
H(1)	11007(14)	2229(11)	6389(12)	83(6)
H(2)	12135(15)	1733(11)	7640(13)	89(7)
H(3)	12207(17)	466(13)	8075(14)	115(8)
H(4)	10869(19)	-313(15)	7143(16)	142(10)
H(5)	9801(12)	190(9)	5760(10)	60(6)
H(7)	8984(11)	1156(8)	4771(10)	48(5)
H(8C)	10557(13)	2000(10)	4625(11)	68(6)
H(8B)	9573(14)	1778(10)	3746(12)	83(6)
H(8A)	10399(14)	1163(11)	4319(12)	82(7)
H(9)	8783(10)	1989(8)	6142(9)	41(4)
H(11A)	9113	3044	7018	104
H(12)	8889(18)	4314(13)	7294(15)	123(9)
H(13)	8070(16)	5146(13)	6199(13)	106(8)
H(14A)	7306	4618	4760	92
H(15)	7415(12)	3362(9)	4468(11)	61(5)
H(18A)	5792	1357	3160	80
H(19)	4891(14)	843(10)	3978(12)	80(6)
H(21)	4805(15)	642(11)	5310(12)	83(7)
H(22)	5528(17)	678(12)	6930(13)	107(8)
H(23A)	7051	1255	7585	91
H(24)	7929(12)	1779(9)	6873(10)	54(5)
H(2A)	14585	2393	6139	79
H(26A)	13961	4594	4669	102
H(27A)	13851	4856	3271	128
H(28A)	14618	4085	2606	112
H(29A)	15379	3013	3299	115
H(30A)	15467	2732	4668	97
H(32)	14438(13)	3867(10)	5931(11)	64(5)
H(33C)	15888(16)	3304(12)	6968(13)	90(8)
H(33B)	16275(15)	3865(12)	6400(13)	89(7)
H(33A)	16280(20)	2966(16)	6245(17)	154(11)
H(34)	13152(10)	2914(8)	4614(9)	40(5)
H(36A)	12978	1642	6204	99
H(37A)	12612	376	5970	136
H(38A)	12331	-145	4625	159
H(39A)	12457	570	3524	143
H(40)	12866(14)	1870(10)	3699(12)	74(6)
H(44)	10801(12)	4214(9)	6248(11)	60(5)
H(46)	9519(15)	4317(11)	4779(12)	93(7)
H(47)	9074(18)	4013(14)	3299(15)	124(9)
H(46)	10160(17)	3344(13)	2755(15)	111(8)
H(49)	11640(13)	2958(10)	3718(11)	63(6)


C4
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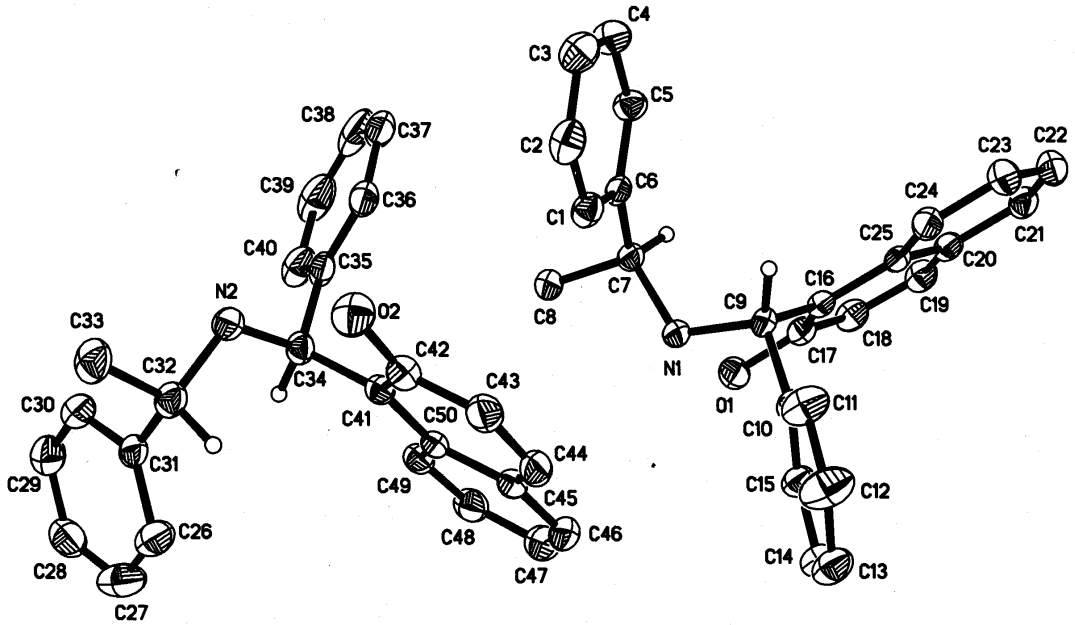
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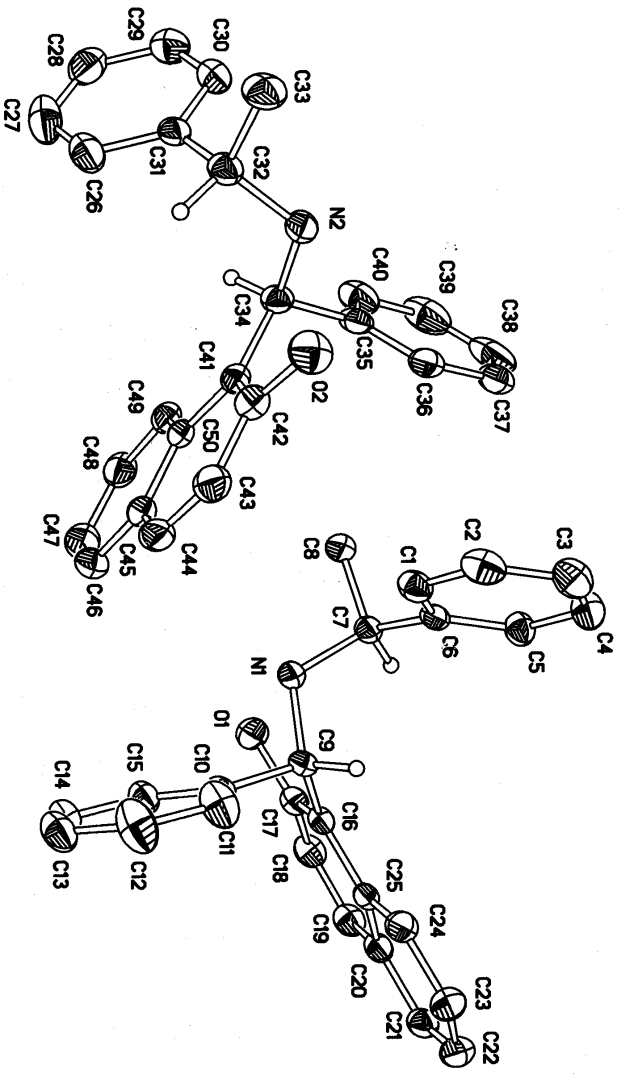
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Table 1. Crystal data and structure refinement for 1zu2.

Identification code	ABC1zu2 (11/8-2000)
Empirical formula	$C_{22}H_{25}NO$
Formula weight	319.43
Temperature	294(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 9.7303(14) Å alpha = 90° b = 10.5655(15) Å beta = 90° c = 35.924(5) Å gamma = 90°
Volume, Z	3693.2(9) $Å^3$, 8
Density (calculated)	1.149 Mg/m^3
Absorption coefficient	0.069 mm^{-1}
F(000)	1376
Crystal size	0.30 x 0.22 x 0.22 mm
θ range for data collection	1.13 to 27.58°
Limiting indices	$-12 \le h \le 12$, $-13 \le k \le 13$, $-46 \le l \le 26$
Reflections collected	25080
Independent reflections	8536 (R_{int} = 0.0513)
Completeness to θ = 27.58°	99.7 %
Absorption correction	SADABS(semi-empirical)
Max. and min. transmission	0.9849 and 0.9795
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8536 / 0 / 514
Goodness-of-fit on F^2	0.739
Final R indices [I>2σ(I)]	R1 = 0.0460, wR2 = 0.1190
R indices (all data)	R1 = 0.1204, wR2 = 0.1551
Absolute structure parameter	-0.1(18)
Extinction coefficient	0.0029(4)

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for lzu2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	-2257(1)	-8887(1)	-2186(1)	68(1)
N(1)	-4427(1)	-9128(1)	-1767(1)	52(1)
C(1)	-4795(2)	-10948(2)	-962(1)	70(1)
C(2)	-5754(2)	-11653(2)	-767(1)	82(1)
C(3)	-7075(2)	-11253(2)	-743(1)	83(1)
C(4)	-7455(2)	-10148(2)	-909(1)	89(1)
C(5)	-6499(2)	-9445(2)	-1104(1)	74(1)
C(6)	-5152(2)	-9825(1)	-1136(1)	53(1)
C(7)	-4136(2)	-9082(1)	-1364(1)	58(1)
C(8)	-4046(2)	-7674(2)	-1246(1)	86(1)
C(9)	-4500(1)	-10411(1)	-1930(1)	45(1)
C(10)	-5338(2)	-10348(1)	-2294(1)	51(1)
C(11)	-6800(2)	-9902(2)	-2222(1)	85(1)
C(12)	-5361(2)	-11602(2)	-2501(1)	68(1)
C(13)	-3055(1)	-10927(1)	-1983(1)	45(1)
C(14)	-2032(2)	-10146(1)	-2116(1)	54(1)
C(15)	-706(2)	-10599(2)	-2192(1)	65(1)
C(16)	-393(2)	-11826(2)	-2131(1)	68(1)
C(17)	-1374(2)	-12675(1)	-1985(1)	55(1)
C(18)	-1045(2)	-13965(2)	-1917(1)	69(1)
C(19)	-1988(2)	-14782(2)	-1777(1)	71(1)
C(20)	-3310(2)	-14352(2)	-1703(1)	68(1)
C(21)	-3666(2)	-13112(1)	-1765(1)	56(1)
C(22)	-2716(1)	-12223(1)	-1910(1)	47(1)
O(2)	-11016(1)	-18058(1)	-765(1)	71(1)
N(2)	-11069(1)	-15865(1)	-427(1)	54(1)
C(23)	-11482(2)	-13055(2)	-257(1)	91(1)
C(24)	-11107(3)	-11796(2)	-230(1)	111(1)
C(25)	-10862(2)	-11102(2)	-537(1)	93(1)
C(26)	-10953(2)	-11668(2)	-870(1)	91(1)
C(27)	-11319(2)	-12937(2)	-906(1)	71(1)
C(28)	-11592(1)	-13636(1)	-597(1)	52(1)
C(29)	-12010(2)	-15017(1)	-621(1)	56(1)
C(30)	-13458(2)	-15227(2)	-472(1)	89(1)
C(31)	-9617(2)	-15812(1)	-551(1)	51(1)
C(32)	-8697(2)	-16509(2)	-266(1)	68(1)
C(33)	-8853(2)	-15925(2)	123(1)	95(1)
C(34)	-7199(2)	-16475(2)	-387(1)	96(1)
C(35)	-9519(1)	-16371(1)	-940(1)	46(1)
C(36)	-10196(2)	-17484(1)	-1023(1)	56(1)
C(37)	-8594(2)	-16401(2)	-1580(1)	55(1)
C(38)	-9305(2)	-17544(2)	-1641(1)	67(1)
C(39)	-10089(2)	-18060(1)	-1371(1)	67(1)
C(40)	-7806(2)	-15823(2)	-1861(1)	73(1)
C(41)	-7166(2)	-14701(2)	-1807(1)	86(1)
C(42)	-7291(2)	-14085(2)	-1467(1)	84(1)
C(43)	-8035(2)	-14605(2)	-1182(1)	65(1)
C(44)	-8721(1)	-15791(1)	-1226(1)	50(1)

Table 3. Bond lengths [Å] and angles [°] for lzu2.

O(1)-C(14)	1.3713(18)	N(1)-C(7)	1.477(2)
N(1)-C(9)	1.4782(17)	C(1)-C(2)	1.384(2)
C(1)-C(6)	1.385(2)	C(2)-C(3)	1.357(3)
C(3)-C(4)	1.361(3)	C(4)-C(5)	1.382(3)
C(5)-C(6)	1.375(2)	C(6)-C(7)	1.504(2)
C(7)-C(8)	1.550(2)	C(9)-C(13)	1.5204(19)
C(9)-C(10)	1.543(2)	C(10)-C(12)	1.519(2)
C(10)-C(11)	1.522(2)	C(13)-C(14)	1.379(2)
C(13)-C(22)	1.4324(19)	C(14)-C(15)	1.403(2)
C(15)-C(16)	1.350(2)	C(16)-C(17)	1.412(2)
C(17)-C(22)	1.416(2)	C(17)-C(18)	1.422(2)
C(18)-C(19)	1.356(2)	C(19)-C(20)	1.390(2)
C(20)-C(21)	1.373(2)	C(21)-C(22)	1.417(2)
O(2)-C(36)	1.3663(19)	N(2)-C(29)	1.4587(19)
N(2)-C(31)	1.4825(19)	C(23)-C(28)	1.370(2)
C(23)-C(24)	1.382(3)	C(24)-C(25)	1.347(3)
C(25)-C(26)	1.340(3)	C(26)-C(27)	1.394(2)
C(27)-C(28)	1.361(2)	C(28)-C(29)	1.516(2)
C(29)-C(30)	1.523(2)	C(31)-C(35)	1.522(2)
C(31)-C(32)	1.545(2)	C(32)-C(34)	1.521(3)
C(32)-C(33)	1.537(3)	C(35)-C(36)	1.3799(19)
C(35)-C(44)	1.426(2)	C(36)-C(39)	1.392(2)
C(37)-C(40)	1.405(2)	C(37)-C(38)	1.409(2)
C(37)-C(44)	1.433(2)	C(38)-C(39)	1.350(2)
C(40)-C(41)	1.353(3)	C(41)-C(42)	1.389(3)
C(42)-C(43)	1.370(2)	C(43)-C(44)	1.428(2)

C(7)-N(1)-C(9)	115.31(11)	C(2)-C(1)-C(6)	121.34(16)
C(3)-C(2)-C(1)	120.23(17)	C(2)-C(3)-C(4)	119.76(18)
C(3)-C(4)-C(5)	120.04(17)	C(6)-C(5)-C(4)	121.77(17)
C(5)-C(6)-C(1)	116.86(15)	C(5)-C(6)-C(7)	121.24(14)
C(1)-C(6)-C(7)	121.84(14)	N(1)-C(7)-C(6)	112.98(12)
N(1)-C(7)-C(8)	108.05(13)	C(6)-C(7)-C(8)	112.95(14)
N(1)-C(9)-C(13)	109.51(11)	N(1)-C(9)-C(10)	108.75(11)
C(13)-C(9)-C(10)	113.46(11)	C(12)-C(10)-C(11)	109.85(13)
C(12)-C(10)-C(9)	112.65(12)	C(11)-C(10)-C(9)	111.23(13)
C(14)-C(13)-C(22)	118.04(12)	C(14)-C(13)-C(9)	119.74(12)
C(22)-C(13)-C(9)	122.19(12)	O(1)-C(14)-C(13)	122.00(13)
O(1)-C(14)-C(15)	116.22(13)	C(13)-C(14)-C(15)	121.77(14)
C(16)-C(15)-C(14)	120.31(15)	C(15)-C(16)-C(17)	121.15(15)
C(16)-C(17)-C(22)	118.73(14)	C(16)-C(17)-C(18)	121.39(14)
C(22)-C(17)-C(18)	119.88(14)	C(19)-C(18)-C(17)	121.45(15)
C(18)-C(19)-C(20)	119.30(15)	C(21)-C(20)-C(19)	120.89(15)
C(20)-C(21)-C(22)	121.87(14)	C(21)-C(22)-C(17)	116.60(13)
C(21)-C(22)-C(13)	123.43(13)	C(17)-C(22)-C(13)	119.96(13)
C(29)-N(2)-C(31)	115.54(11)	C(28)-C(23)-C(24)	121.05(19)
C(25)-C(24)-C(23)	120.8(2)	C(26)-C(25)-C(24)	118.53(18)
C(25)-C(26)-C(27)	121.94(19)	C(28)-C(27)-C(26)	119.73(18)
C(27)-C(28)-C(23)	117.95(15)	C(27)-C(28)-C(29)	121.87(15)
C(23)-C(28)-C(29)	120.19(15)	N(2)-C(29)-C(28)	113.34(12)
N(2)-C(29)-C(30)	108.89(13)	C(28)-C(29)-C(30)	111.59(13)
N(2)-C(31)-C(35)	108.72(12)	N(2)-C(31)-C(32)	109.60(12)
C(35)-C(31)-C(32)	112.73(12)	C(34)-C(32)-C(33)	110.19(16)
C(34)-C(32)-C(31)	110.81(15)	C(33)-C(32)-C(31)	110.68(14)
C(36)-C(35)-C(44)	118.05(14)	C(36)-C(35)-C(31)	120.02(13)

C(44)-C(35)-C(31)	121.92(12)	O(2)-C(36)-C(35)	120.65(14)
O(2)-C(36)-C(39)	117.26(13)	C(35)-C(36)-C(39)	122.09(15)
C(40)-C(37)-C(38)	122.02(15)	C(40)-C(37)-C(44)	119.26(14)
C(38)-C(37)-C(44)	118.68(14)	C(39)-C(38)-C(37)	120.90(15)
C(38)-C(39)-C(36)	120.64(15)	C(41)-C(40)-C(37)	122.03(16)
C(40)-C(41)-C(42)	119.68(18)	C(43)-C(42)-C(41)	121.08(18)
C(42)-C(43)-C(44)	121.05(16)	C(35)-C(44)-C(43)	123.51(14)
C(35)-C(44)-C(37)	119.58(13)	C(43)-C(44)-C(37)	116.90(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for lzu2.

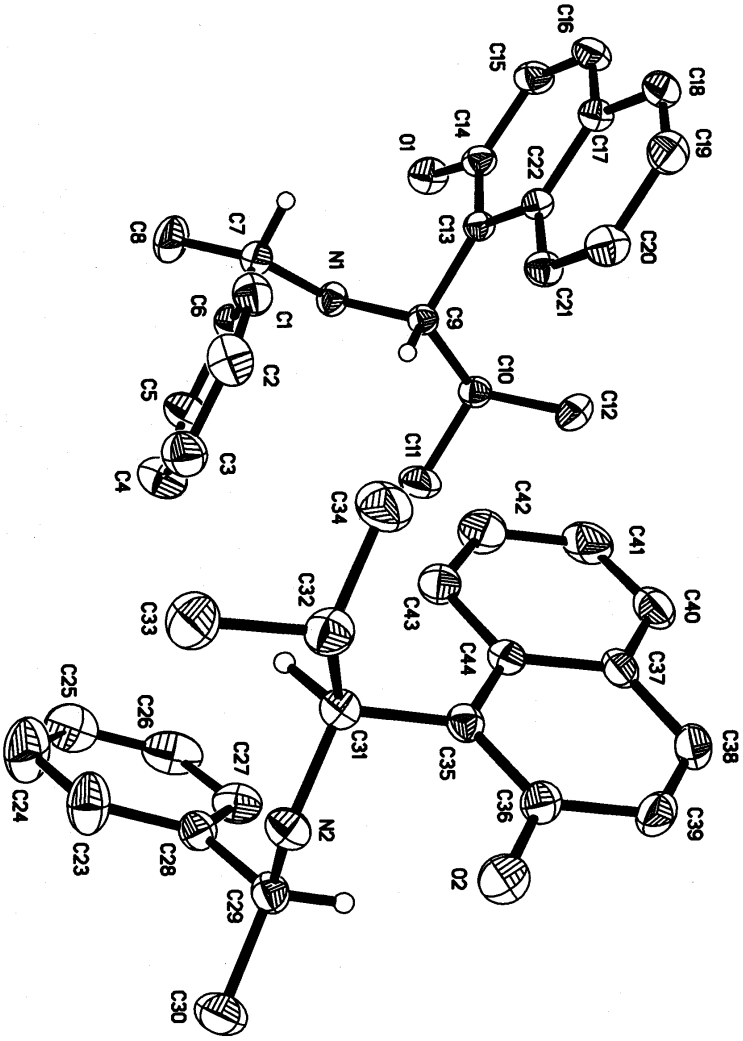
The anisotropic displacement factor exponent takes the form:

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

	U11	U22	U33	U23	U13	U12
O(1)	69(1)	54(1)	82(1)	13(1)	3(1)	-12(1)
N(1)	57(1)	45(1)	52(1)	-3(1)	-4(1)	4(1)
C(1)	76(1)	72(1)	62(1)	3(1)	-4(1)	18(1)
C(2)	103(1)	74(1)	70(1)	18(1)	8(1)	13(1)
C(3)	82(1)	97(1)	69(1)	8(1)	10(1)	-4(1)
C(4)	65(1)	107(1)	95(1)	15(1)	10(1)	5(1)
C(5)	63(1)	73(1)	87(1)	13(1)	8(1)	10(1)
C(6)	54(1)	58(1)	47(1)	-6(1)	-2(1)	5(1)
C(7)	55(1)	58(1)	61(1)	-12(1)	-5(1)	4(1)
C(8)	110(1)	60(1)	89(1)	-25(1)	0(1)	-14(1)
C(9)	43(1)	44(1)	48(1)	-1(1)	3(1)	-2(1)
C(10)	48(1)	54(1)	50(1)	4(1)	-1(1)	-1(1)
C(11)	48(1)	124(2)	83(1)	-7(1)	-9(1)	18(1)
C(12)	73(1)	69(1)	63(1)	-5(1)	-16(1)	-7(1)
C(13)	41(1)	48(1)	44(1)	-1(1)	0(1)	-3(1)
C(14)	47(1)	61(1)	54(1)	1(1)	0(1)	-7(1)
C(15)	48(1)	77(1)	70(1)	6(1)	6(1)	-10(1)
C(16)	43(1)	87(1)	73(1)	-4(1)	9(1)	5(1)
C(17)	47(1)	62(1)	56(1)	-4(1)	-3(1)	6(1)
C(18)	59(1)	72(1)	75(1)	-10(1)	-10(1)	22(1)
C(19)	79(1)	57(1)	79(1)	1(1)	-12(1)	13(1)
C(20)	68(1)	57(1)	80(1)	13(1)	-9(1)	1(1)
C(21)	51(1)	53(1)	63(1)	6(1)	-2(1)	2(1)
C(22)	44(1)	52(1)	46(1)	-4(1)	-4(1)	3(1)
O(2)	78(1)	48(1)	87(1)	9(1)	11(1)	-13(1)
N(2)	54(1)	50(1)	59(1)	14(1)	11(1)	0(1)
C(23)	143(2)	55(1)	74(1)	-3(1)	18(1)	-5(1)
C(24)	161(2)	55(1)	116(2)	-21(1)	22(2)	-7(1)
C(25)	90(1)	49(1)	140(2)	6(1)	9(1)	0(1)
C(26)	72(1)	81(1)	122(2)	45(1)	5(1)	-4(1)
C(27)	61(1)	77(1)	75(1)	17(1)	-5(1)	2(1)
C(28)	55(1)	48(1)	55(1)	1(1)	2(1)	4(1)
C(29)	56(1)	54(1)	57(1)	-6(1)	5(1)	5(1)
C(30)	58(1)	75(1)	135(2)	-17(1)	21(1)	-3(1)
C(31)	51(1)	48(1)	52(1)	4(1)	2(1)	1(1)
C(32)	68(1)	70(1)	67(1)	4(1)	-10(1)	7(1)
C(33)	95(1)	127(2)	64(1)	-5(1)	-14(1)	11(1)
C(34)	69(1)	135(2)	84(1)	-3(1)	-13(1)	29(1)
C(35)	45(1)	41(1)	52(1)	1(1)	0(1)	6(1)
C(36)	58(1)	43(1)	68(1)	-2(1)	-3(1)	5(1)
C(37)	47(1)	66(1)	53(1)	-6(1)	3(1)	14(1)
C(38)	67(1)	69(1)	66(1)	-19(1)	0(1)	13(1)
C(39)	67(1)	47(1)	87(1)	-16(1)	-13(1)	1(1)
C(40)	58(1)	105(1)	56(1)	-10(1)	7(1)	17(1)
C(41)	65(1)	119(2)	72(1)	13(1)	23(1)	-11(1)
C(42)	76(1)	92(1)	82(1)	3(1)	22(1)	-25(1)
C(43)	59(1)	68(1)	69(1)	-4(1)	13(1)	-13(1)
C(44)	41(1)	53(1)	56(1)	-2(1)	1(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for lzu2.

	x	y	z	U(eq)
H(1N)	-5300(15)	-8777(12)	-1827(4)	65(4)
H(1)	-3851(17)	-11296(15)	-965(5)	96(6)
H(2)	-5290(20)	-12326(17)	-613(5)	111(6)
H(3)	-7653(19)	-11709(16)	-577(5)	107(6)
H(4)	-8490(20)	-9900(20)	-881(7)	154(9)
H(5A)	-6773	-8695	-1217	89
H(7)	-3310(14)	-9539(13)	-1340(4)	60(4)
H(9)	-5051(12)	-10939(11)	-1754(3)	42(3)
H(10)	-4922(13)	-9695(11)	-2457(3)	45(4)
H(11A)	-7381	-10539	-2074	93(6)
H(11B)	-6754	-9124	-2084	112
H(11C)	-7255	-9727	-2453	112
H(12A)	-5782	-11555	-2745	79(5)
H(12B)	-4439	-11912	-2527	95
H(12C)	-5862	-12196	-2351	95
H(15A)	-40	-10051	-2284	78
H(16)	497(14)	-12190(12)	-2186(4)	58(4)
H(18A)	-164	-14256	-1969	82
H(19A)	-1752	-15620	-1731	86
H(20)	-4016(16)	-14994(14)	-1572(4)	76(5)
H(21)	-4653(14)	-12826(12)	-1689(4)	58(4)
H(2A)	-11339	-16363	-252	65
H(23)	-11700(20)	-13660(19)	-17(5)	120(7)
H(24A)	-11024	-11424	4	133
H(25)	-10550(20)	-10251(18)	-493(5)	111(6)
H(26A)	-10766	-11199	-1083	110
H(27A)	-11377	-13305	-1141	85
H(29)	-11994(14)	-15303(13)	-859(4)	59(4)
H(30A)	-13501	-14833	-204	108(7)
H(30B)	-14136	-14836	-629	130
H(30C)	-13650	-16117	-460	130
H(31)	-9285(14)	-14794(12)	-534(4)	57(4)
H(32)	-9034(17)	-17491(15)	-261(5)	85(5)
H(33A)	-9801	-15956	197	143
H(33B)	-8550	-15061	118	143
H(33C)	-8307	-16394	298	143
H(34A)	-6488	-16679	-212	155(9)
H(34B)	-7099	-17038	-595	186
H(34C)	-7021	-15636	-477	186
H(38)	-9205(17)	-17976(15)	-1885(5)	88(5)
H(39A)	-10564	-18808	-1417	80
H(40)	-7690(15)	-16209(14)	-2081(4)	73(5)
H(41A)	-6644	-14344	-1997	103
H(42A)	-6863	-13307	-1433	100
H(43)	-8124(14)	-14159(13)	-930(4)	64(4)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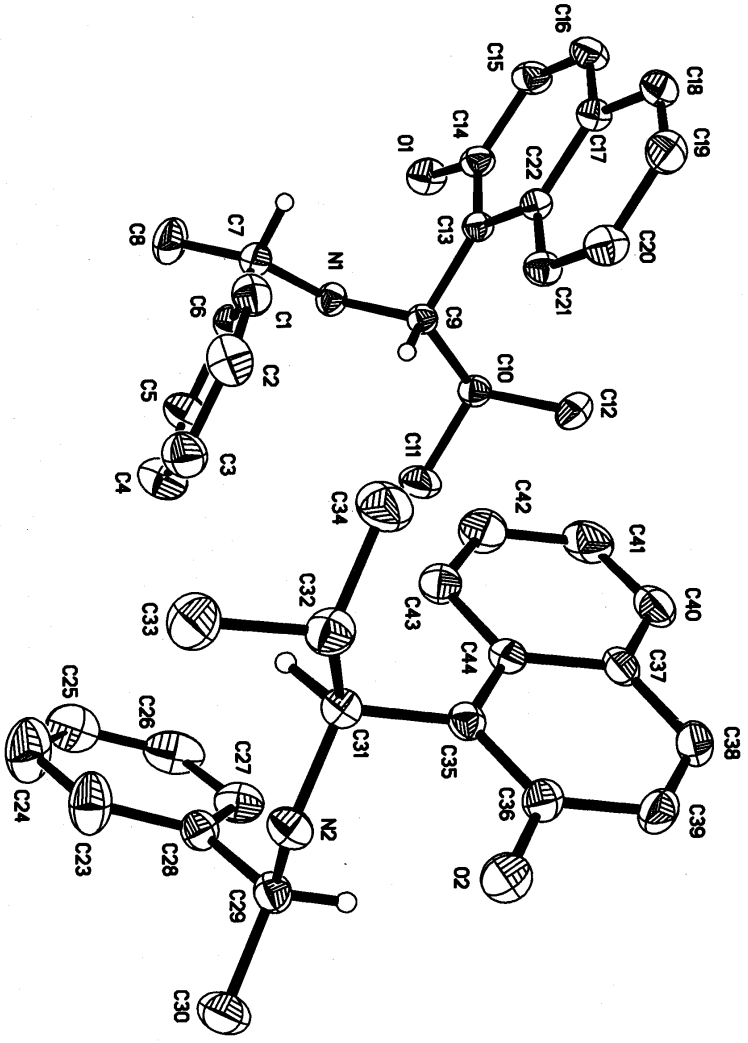
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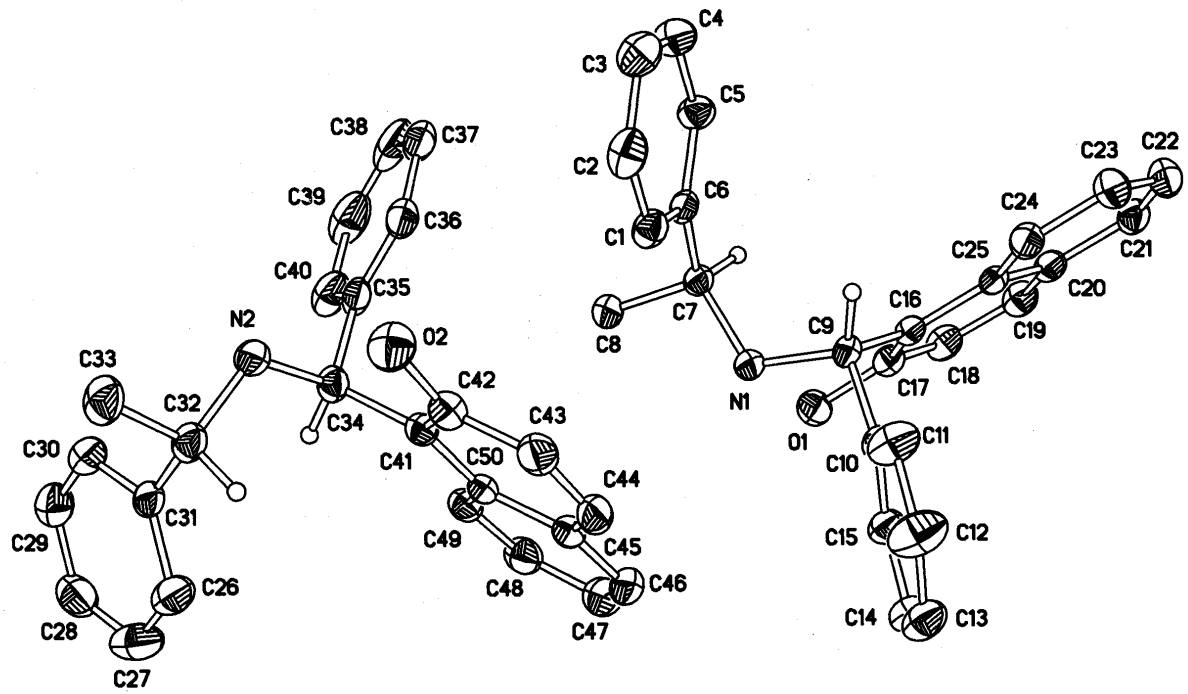
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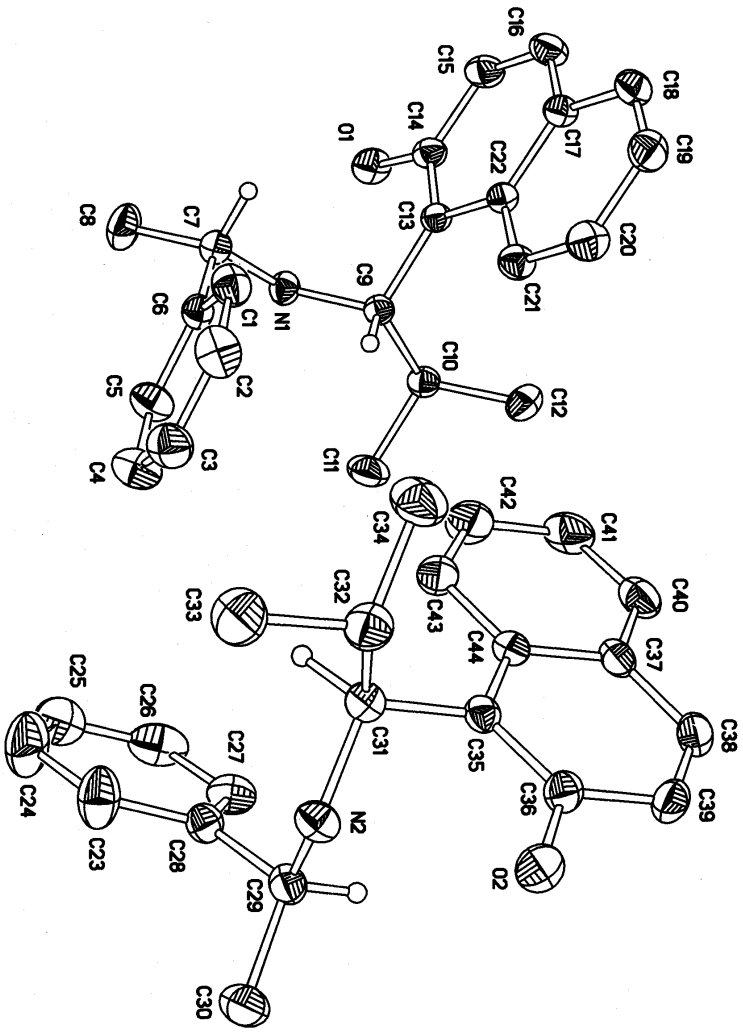
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