Supporting information for:

An Improved Mimetic Compound for Styrene "Living" Free Radical Polymerization. An Initiator Containing the "Penultimate" Unit

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Notes:

file ts001 refers to compound **2**

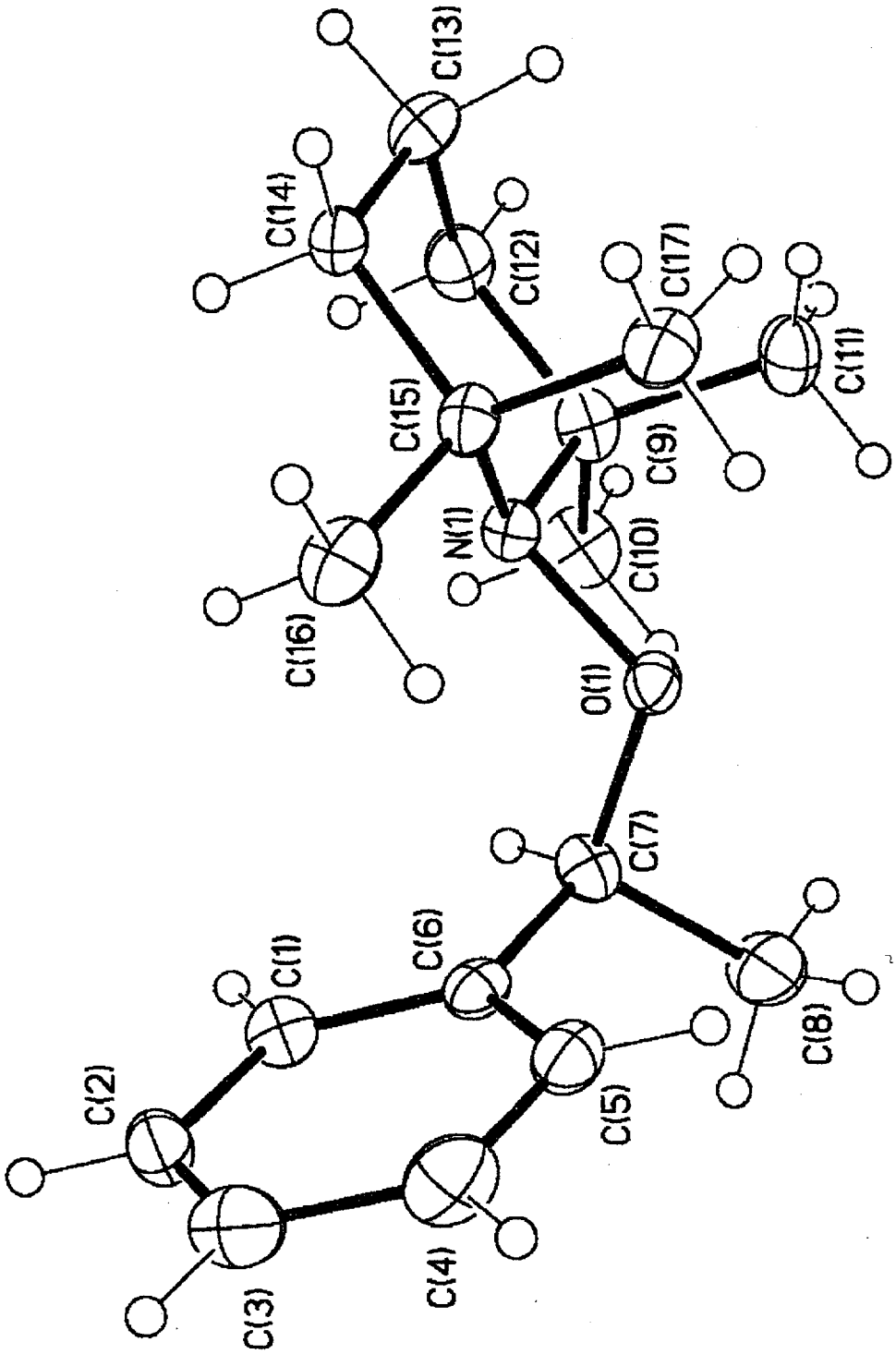
file ts002 refers to compound **4**

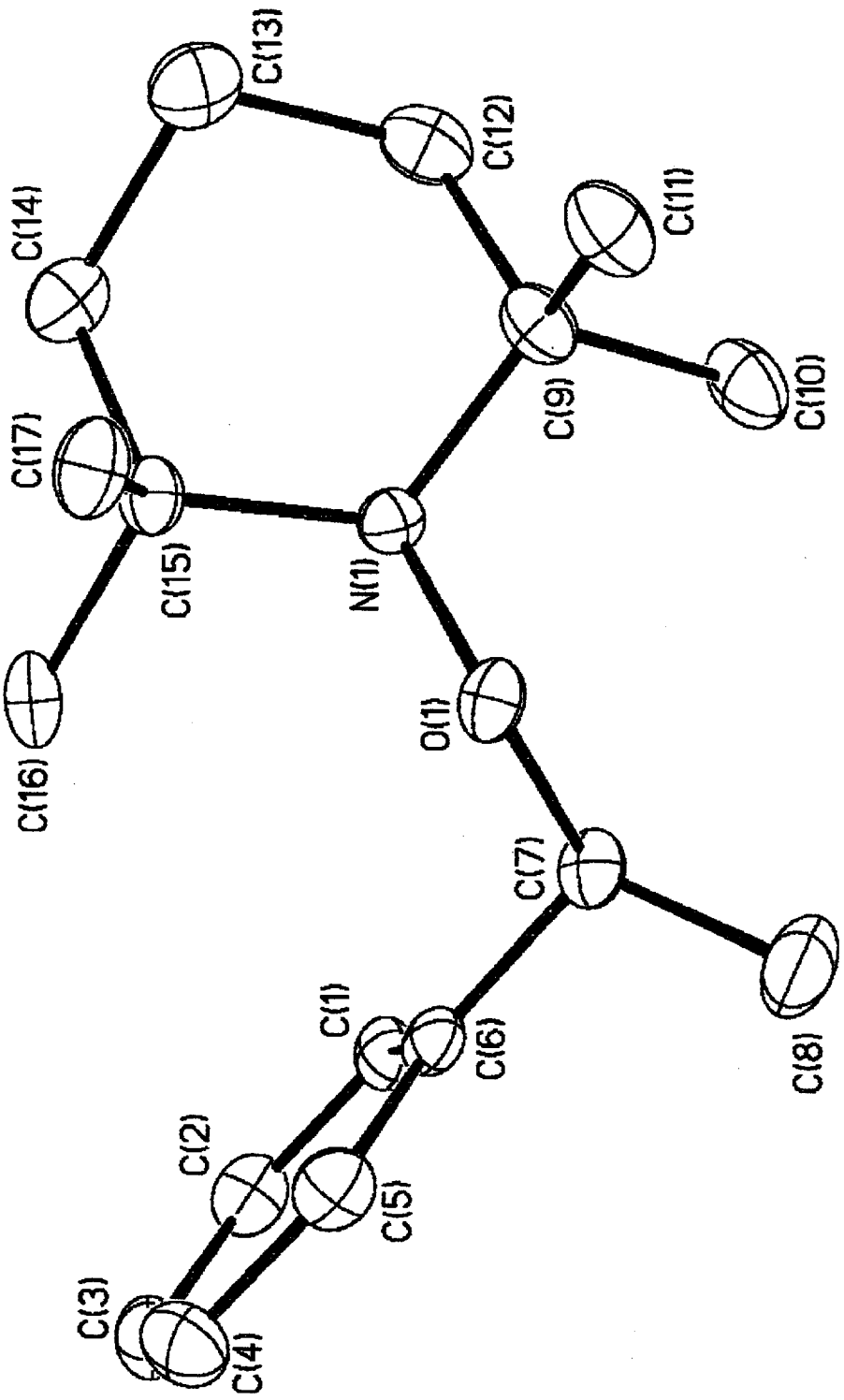
Supporting information

Data for Figure 1

Decomposition kinetices for initiators 2 and 4.

Compound	T (°C)	k/s^{-1}
2	76	2.89×10^{-6}
2	79	4.79×10^{-6}
2	90	1.45×10^{-5}
2	103	5.77×10^{-5}
2	114	2.16×10^{-4}
2	119	4.98×10^{-4}
4	76.2	5.1×10^{-7}
4	93.5	5.1×10^{-6}
4	117.5	6.6×10^{-5}





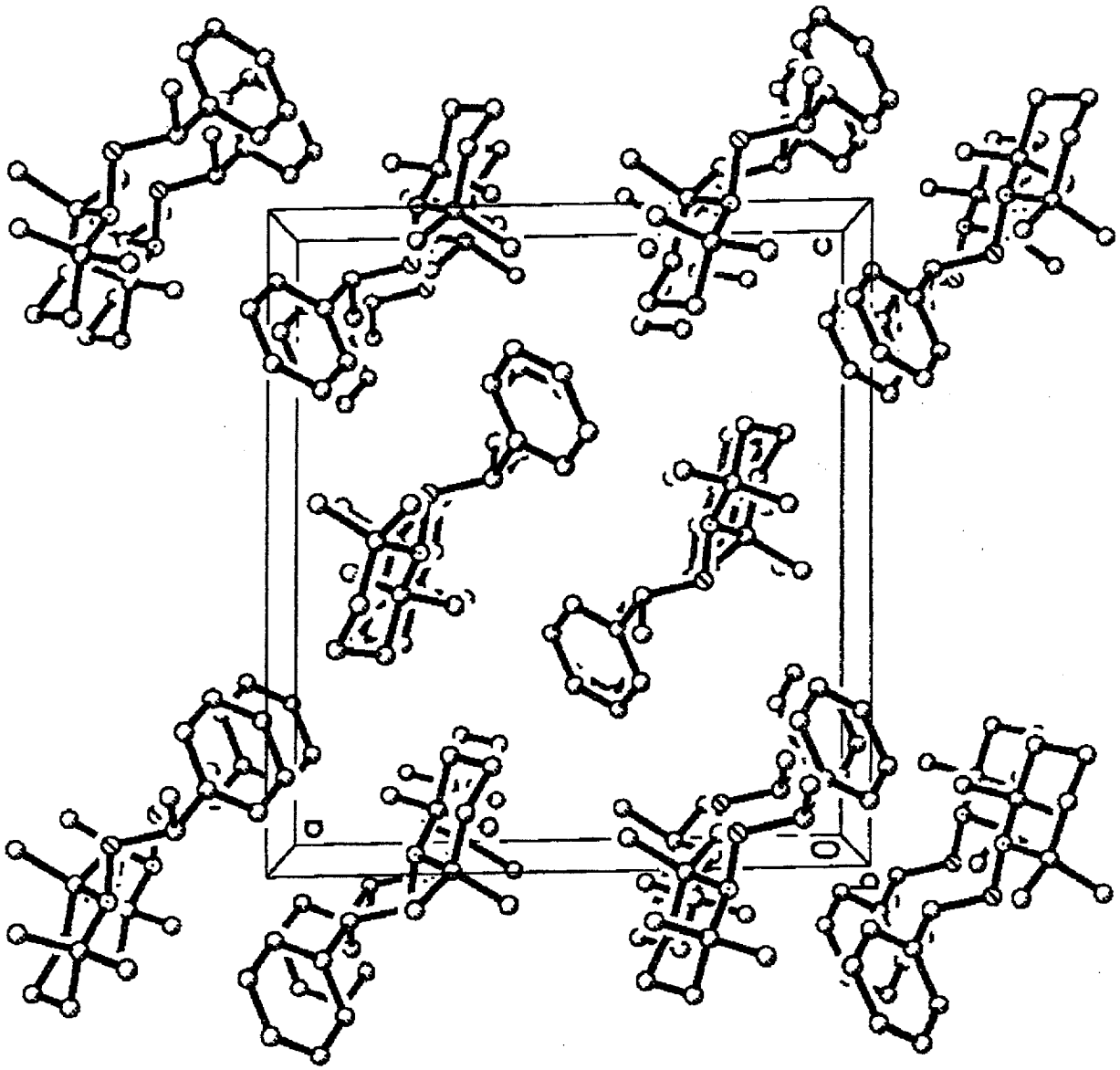


Table 1. Crystal data and structure refinement for ts001.

Identification code	ts001
Empirical formula	C17 H27 N O
Formula weight	261.40
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 13.534(9) A alpha = 90 deg. b = 7.705(8) A beta = 91.61(3) deg. c = 14.921(9) A gamma = 90 deg.
Volume	1556(1) A^3
Z, Calculated density	4, 1.116 Mg/m^3
Absorption coefficient	0.068 mm^-1
F(000)	576
Crystal size	.3 x .2 x .2 mm
Theta range for data collection	2.06 to 28.53 deg.
Limiting indices	-14<=h<=13, 0<=k<=10, 0<=l<=19
Reflections collected / unique	4436 / 2924 [R(int) = 0.1058]
Completeness to theta = 28.53	73.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2924 / 0 / 160
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0668, wR2 = 0.1287
R indices (all data)	R1 = 0.1967, wR2 = 0.1445
Largest diff. peak and hole	0.247 and -0.280 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ts001.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	7281(2)	1523(3)	5698(2)	31(1)
N(1)	7406(2)	2390(4)	4835(2)	27(1)
C(1)	5072(2)	3767(3)	6037(1)	35(1)
C(2)	4707(2)	5192(3)	6493(2)	44(1)
C(3)	5110(2)	5642(3)	7328(2)	48(1)
C(4)	5878(2)	4666(4)	7707(1)	50(1)
C(5)	6244(2)	3241(3)	7250(2)	39(1)
C(6)	5841(2)	2792(3)	6415(2)	30(1)
C(7)	6243(3)	1285(4)	5907(2)	31(1)
C(8)	6218(3)	-394(5)	6448(3)	55(1)
C(9)	7745(3)	1032(5)	4208(2)	35(1)
C(10)	6890(3)	-215(5)	4018(2)	48(1)
C(11)	8631(3)	-52(4)	4539(2)	45(1)
C(12)	7976(3)	1951(5)	3331(2)	47(1)
C(13)	8718(3)	3417(5)	3446(3)	49(1)
C(14)	8299(3)	4687(5)	4107(2)	40(1)
C(15)	8062(3)	3920(4)	5011(2)	30(1)
C(16)	7476(3)	5271(4)	5520(2)	43(1)
C(17)	9007(3)	3535(4)	5568(2)	40(1)

Table 3. Bond lengths [A] and angles [deg] for cs001.

O(1)-C(7)	1.459(4)
O(1)-N(1)	1.465(4)
N(1)-C(9)	1.485(4)
N(1)-C(15)	1.494(4)
C(1)-C(2)	1.3900
C(1)-C(6)	1.3900
C(2)-C(3)	1.3900
C(3)-C(4)	1.3900
C(4)-C(5)	1.3900
C(5)-C(6)	1.3900
C(6)-C(7)	1.498(4)
C(7)-C(8)	1.525(5)
C(9)-C(10)	1.525(5)
C(9)-C(12)	1.528(5)
C(9)-C(11)	1.532(5)
C(12)-C(13)	1.517(5)
C(13)-C(14)	1.511(5)
C(14)-C(15)	1.515(5)
C(15)-C(16)	1.525(5)
C(15)-C(17)	1.535(5)

C(7)-O(1)-N(1)	112.4(2)
O(1)-N(1)-C(9)	106.1(3)
O(1)-N(1)-C(15)	106.7(3)
C(9)-N(1)-C(15)	118.3(3)
C(2)-C(1)-C(6)	120.0
C(1)-C(2)-C(3)	120.0
C(4)-C(3)-C(2)	120.0
C(5)-C(4)-C(3)	120.0
C(6)-C(5)-C(4)	120.0
C(5)-C(6)-C(1)	120.0
C(5)-C(6)-C(7)	120.5(3)
C(1)-C(6)-C(7)	119.5(3)
O(1)-C(7)-C(6)	112.1(3)
O(1)-C(7)-C(8)	104.8(3)
C(6)-C(7)-C(8)	112.1(3)
N(1)-C(9)-C(10)	108.3(3)
N(1)-C(9)-C(12)	106.7(3)
C(10)-C(9)-C(12)	107.8(3)
N(1)-C(9)-C(11)	115.7(3)
C(10)-C(9)-C(11)	107.5(3)
C(12)-C(9)-C(11)	110.6(3)
C(13)-C(12)-C(9)	113.5(3)
C(14)-C(13)-C(12)	107.3(3)
C(13)-C(14)-C(15)	114.9(3)
N(1)-C(15)-C(14)	106.9(3)
N(1)-C(15)-C(16)	108.1(3)
C(14)-C(15)-C(16)	107.7(3)
N(1)-C(15)-C(17)	115.2(3)
C(14)-C(15)-C(17)	111.3(3)
C(16)-C(15)-C(17)	107.4(3)

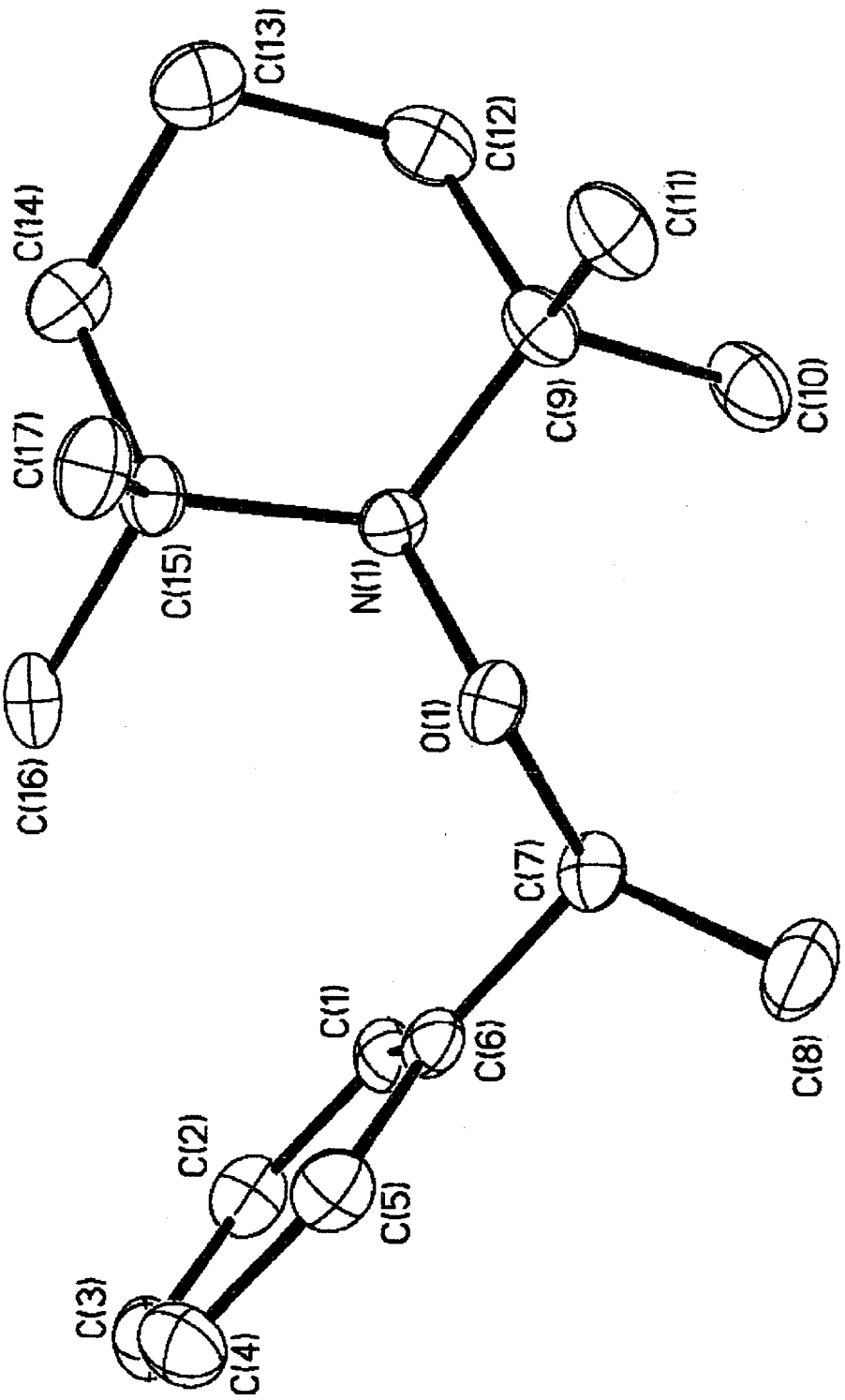
Symmetry transformations used to generate equivalent atoms:

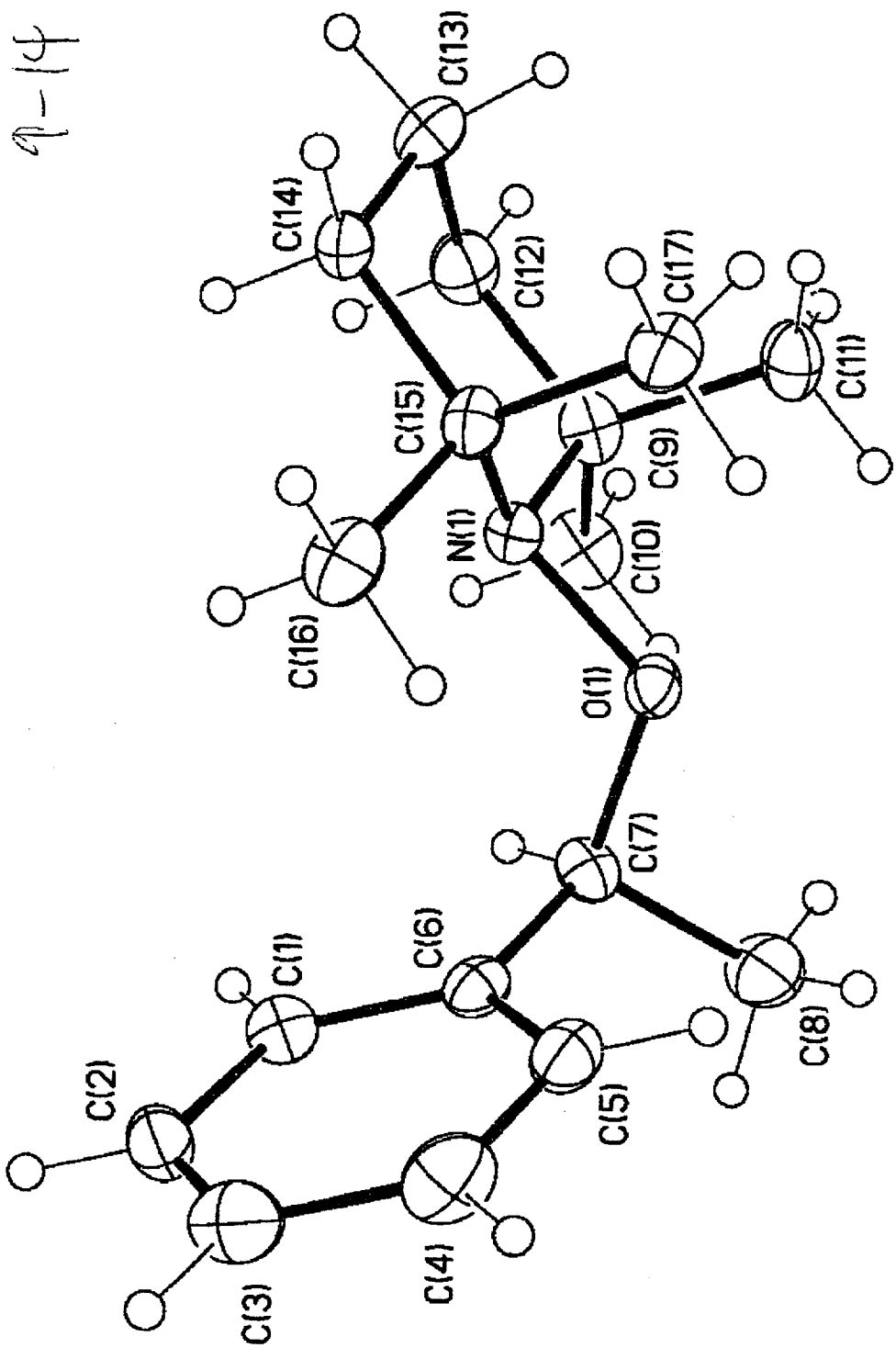
Table 4. Anisotropic displacement parameters (A 2 x 10 3) for [illegible].
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

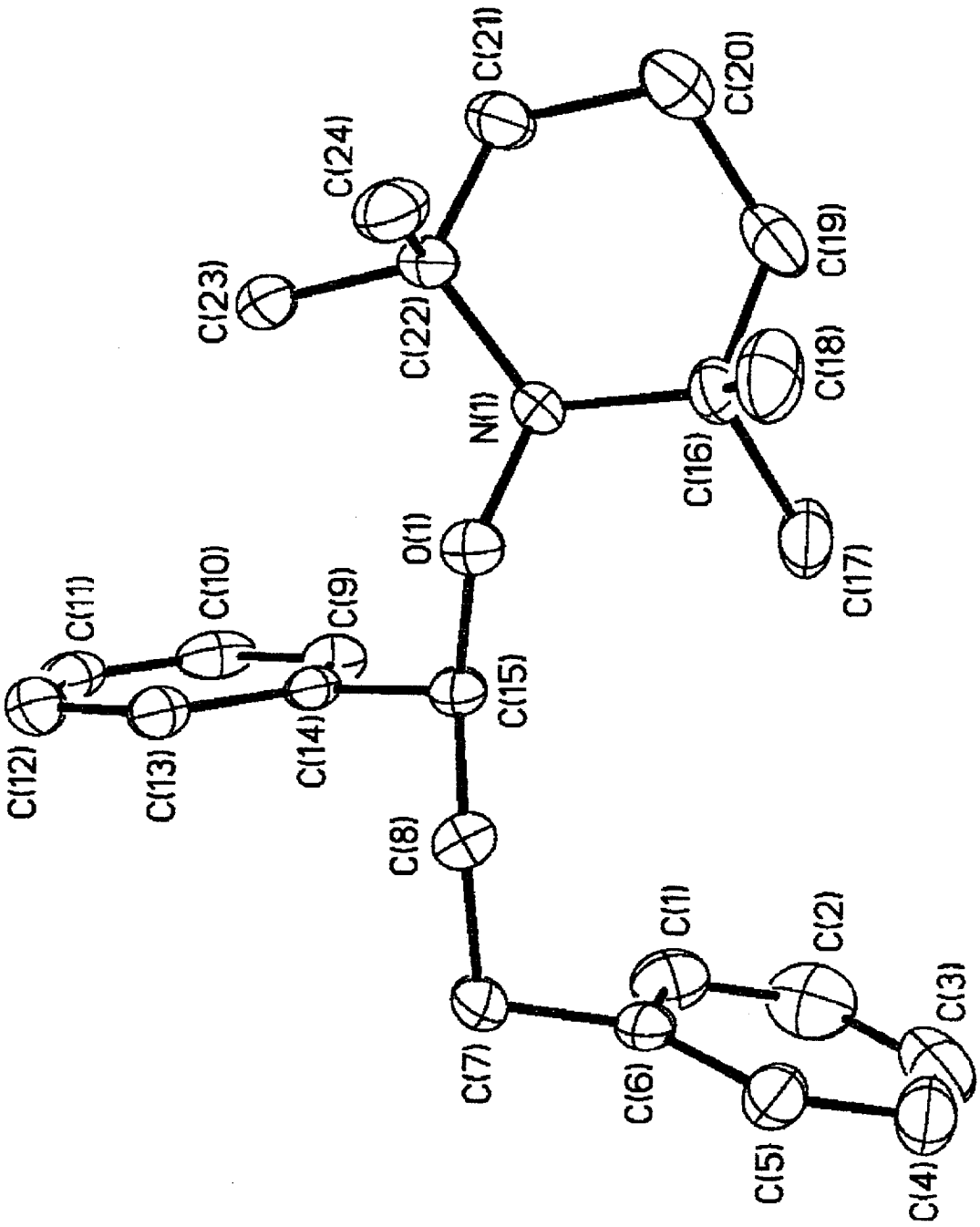
	U11	U22	U33	U23	U13	U12
O(1)	27(2)	28(2)	37(2)	5(1)	-6(1)	-3(1)
N(1)	27(2)	27(2)	27(2)	3(2)	1(2)	2(2)
C(1)	30(3)	33(3)	41(3)	-3(2)	-1(2)	-8(2)
C(2)	34(3)	42(3)	56(3)	8(2)	2(3)	5(2)
C(3)	50(4)	38(3)	58(3)	-8(2)	9(3)	-9(2)
C(4)	62(4)	53(3)	36(3)	-6(2)	-6(3)	-6(3)
C(5)	37(3)	42(3)	36(3)	6(2)	-4(2)	-1(2)
C(6)	27(3)	33(2)	31(2)	2(2)	1(2)	-10(2)
C(7)	19(3)	32(2)	41(2)	-1(2)	-5(2)	-4(2)
C(8)	52(3)	35(2)	78(3)	13(2)	17(3)	-5(2)
C(9)	36(3)	36(2)	31(2)	-7(2)	-7(2)	4(2)
C(10)	45(3)	47(3)	52(3)	-21(2)	-6(2)	-3(2)
C(11)	55(3)	36(3)	44(3)	-4(2)	-3(2)	11(2)
C(12)	49(3)	53(3)	37(3)	-6(2)	-1(2)	9(2)
C(13)	55(3)	52(3)	38(3)	14(2)	4(2)	1(3)
C(14)	35(3)	39(2)	46(3)	13(2)	0(2)	4(2)
C(15)	28(3)	28(2)	34(2)	0(2)	-5(2)	-2(2)
C(16)	50(3)	24(2)	55(3)	-4(2)	-4(2)	-10(2)
C(17)	34(3)	38(3)	48(3)	2(2)	-7(2)	-9(2)

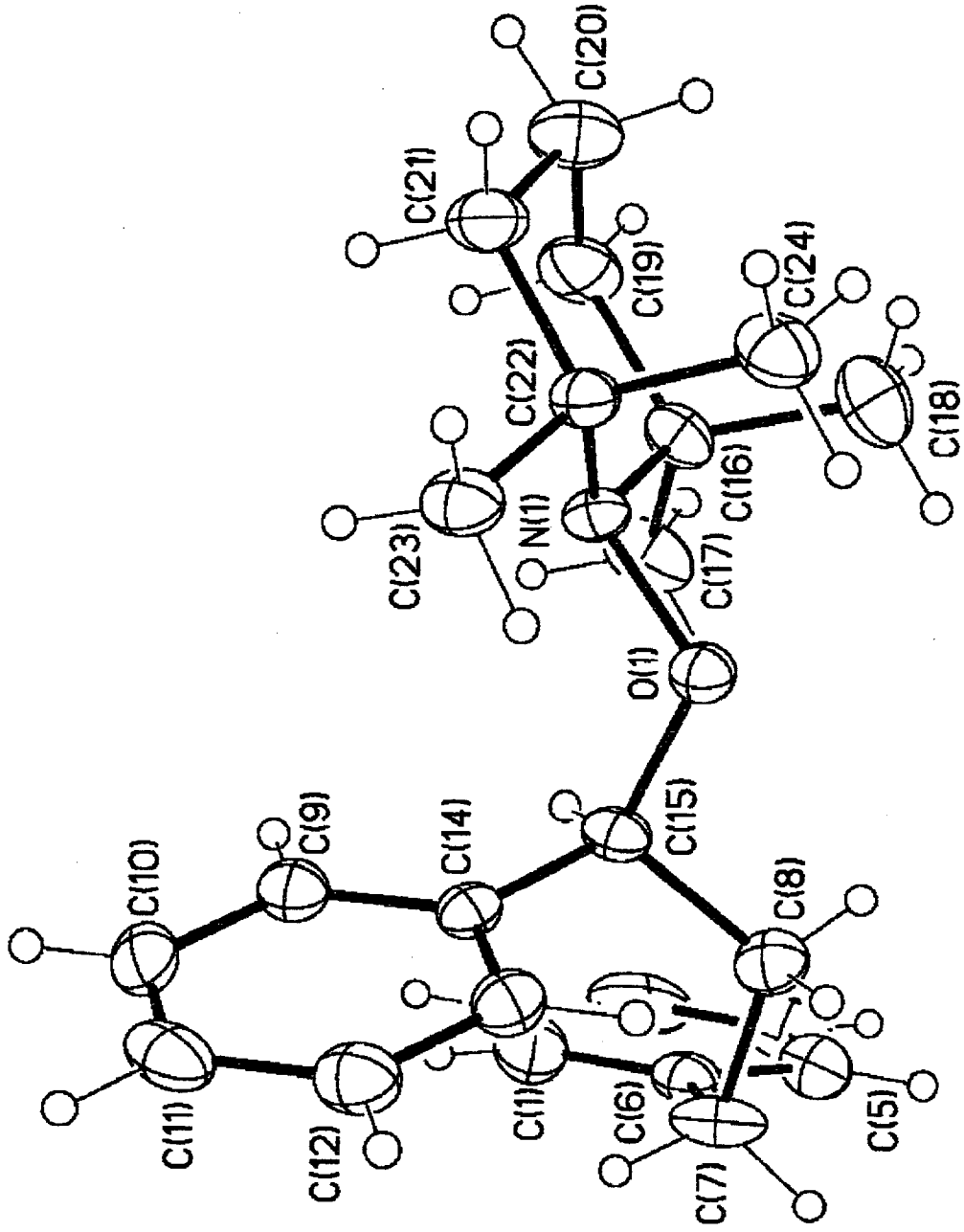
Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ts001.

	x	y	z	U(eq)
H(1A)	4800	3463	5472	42
H(2A)	4188	5851	6237	53
H(3A)	4863	6605	7636	58
H(4A)	6151	4970	8271	60
H(5A)	6763	2582	7506	46
H(7A)	5851	1131	5343	37
H(8A)	6448	-1347	6084	82
H(8B)	5547	-623	6626	82
H(8C)	6644	-280	6978	82
H(10A)	6316	433	3803	72
H(10B)	6731	-823	4565	72
H(10C)	7078	-1048	3566	72
H(11A)	8477	-604	5102	68
H(11B)	9202	696	4627	68
H(11C)	8775	-934	4098	68
H(12A)	8236	1098	2911	56
H(12B)	7361	2419	3066	56
H(13A)	9354	2965	3673	58
H(13B)	8821	3990	2870	58
H(14A)	7694	5192	3842	48
H(14B)	8776	5633	4201	48
H(16A)	6869	5537	5186	65
H(16B)	7868	6319	5592	65
H(16C)	7318	4817	6105	65
H(17A)	9392	2660	5267	60
H(17B)	8832	3114	6155	60
H(17C)	9394	4589	5634	60


C(13)
C(12)
C(14)
C(11)
C(17)
C(9)
C(10)
C(15)
N(1)
C(16)
O(1)
C(7)
C(1)
C(6)
C(8)
C(2)
C(5)
C(3)
C(4)




C(21)
C(20)
C(24)
C(19)
C(23)
C(22)
C(18)
N(1)
C(16)
O(1)
C(17)
C(11)
C(10)
C(9)
C(15)
C(12)
C(13)
C(14)
C(8)
C(1)
C(2)
C(3)
C(7)
C(6)
C(5)
C(4)


C(20)
C(21)
C(19)
C(24)
C(22)
C(18)
C(16)
C(23)
N(1)
C(17)
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C(15)
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C(12)
C(1)
C(6)
C(5)
C(7)

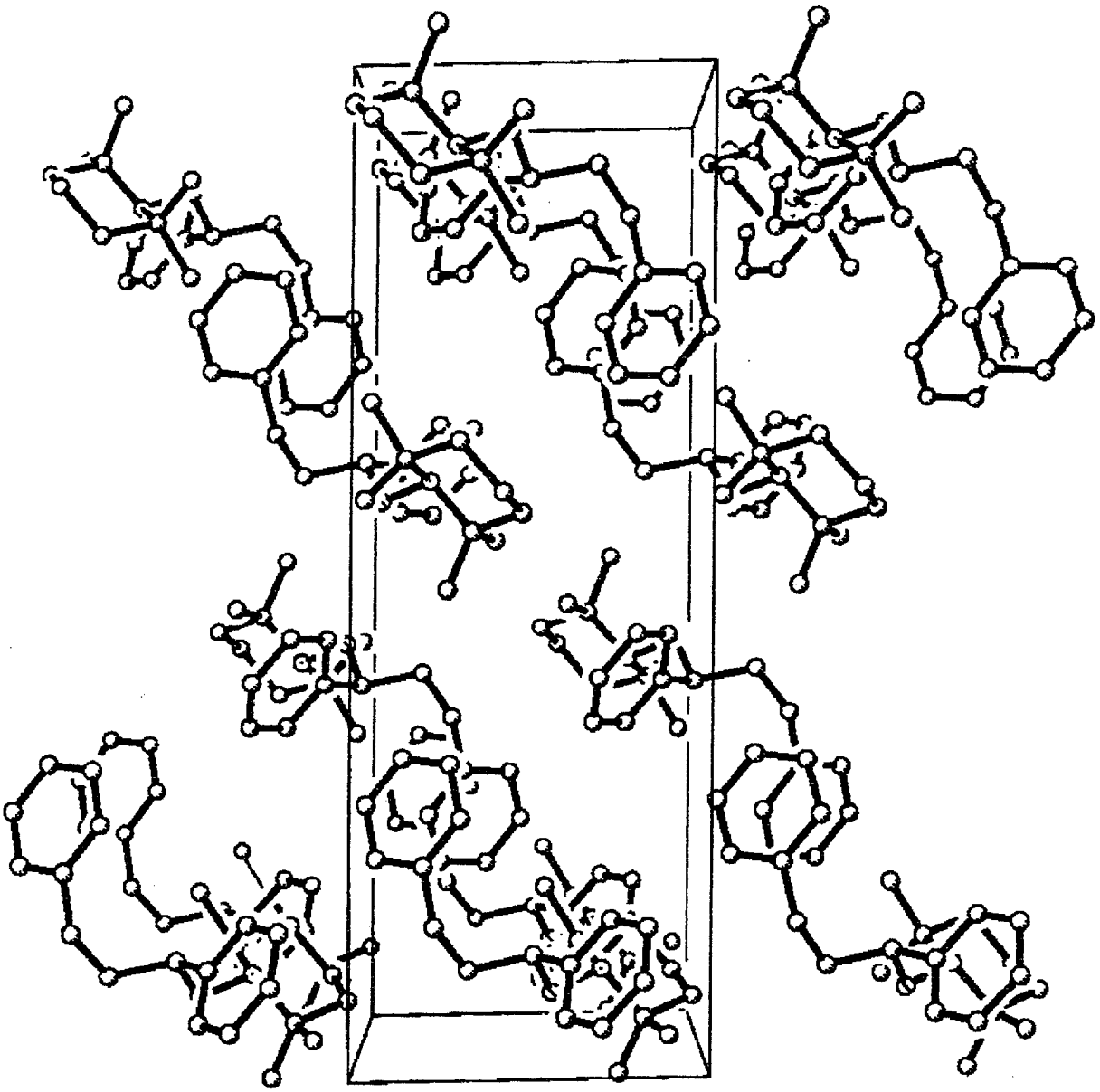

Table 1. Crystal data and structure refinement.

Identification code	ts002
Empirical formula	C24 H33 N O
Formula weight	351.51
Temperature	203(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 8.078(3) A alpha = 90 deg. b = 11.473(3) A beta = 91.67(3) deg. c = 22.594(6) A gamma = 90 deg.
Volume	2093(1) A^3
Z, Calculated density	4, 1.115 Mg/m^3
Absorption coefficient	0.067 mm^-1
F(000)	768
Crystal size	0.1 x 0.1 x 0.1 mm
Theta range for data collection	1.80 to 28.60 deg.
Limiting indices	-10<=h<=10, 0<=k<=15, 0<=l<=29
Reflections collected / unique	11568 / 4592 [R(int) = 0.1006]
Completeness to theta = 28.60	85.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4592 / 0 / 212
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1207
R indices (all data)	R1 = 0.1785, wR2 = 0.1409
Extinction coefficient	0.0049(9)
Largest diff. peak and hole	0.250 and -0.218 e.A^-3

Table 2. Atomic coordinates (x 10 4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ts002. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	2939(2)	7514(2)	946(1)	37(1)
O(1)	4371(2)	8181(1)	750(1)	41(1)
C(1)	6950(2)	9496(2)	2570(1)	64(1)
C(2)	7287(3)	8893(2)	3094(1)	84(1)
C(3)	8660(4)	8165(2)	3141(1)	84(1)
C(4)	9696(3)	8040(2)	2664(1)	74(1)
C(5)	9359(2)	8643(2)	2141(1)	52(1)
C(6)	7986(3)	9371(2)	2094(1)	42(1)
C(7)	7641(3)	10005(2)	1515(1)	52(1)
C(8)	6729(3)	9250(2)	1049(1)	45(1)
C(9)	2771(2)	10421(2)	1589(1)	46(1)
C(10)	1807(2)	11424(2)	1561(1)	57(1)
C(11)	1943(2)	12187(1)	1086(1)	58(1)
C(12)	3042(3)	11946(1)	640(1)	53(1)
C(13)	4005(2)	10943(2)	669(1)	43(1)
C(14)	3870(2)	10180(1)	1143(1)	36(1)
C(15)	4892(3)	9067(2)	1178(1)	38(1)
C(16)	3586(3)	6363(2)	1169(1)	45(1)
C(17)	4574(4)	6572(2)	1750(1)	65(1)
C(18)	4696(4)	5689(2)	747(1)	67(1)
C(19)	2051(4)	5638(2)	1325(1)	63(1)
C(20)	810(4)	5515(2)	803(2)	67(1)
C(21)	279(3)	6726(2)	601(1)	55(1)
C(22)	1724(3)	7495(2)	434(1)	39(1)
C(23)	1078(3)	8733(2)	339(1)	47(1)
C(24)	2419(3)	7088(2)	-161(1)	54(1)

Table 3. Bond lengths [A] and angles [deg] for ts002.

N(1)-O(1)	1.466(2)
N(1)-C(22)	1.495(3)
N(1)-C(16)	1.502(3)
O(1)-C(15)	1.458(3)
C(1)-C(2)	1.3900
C(1)-C(6)	1.3900
C(2)-C(3)	1.3900
C(3)-C(4)	1.3900
C(4)-C(5)	1.3900
C(5)-C(6)	1.3900
C(6)-C(7)	1.516(3)
C(7)-C(8)	1.535(3)
C(8)-C(15)	1.535(3)
C(9)-C(10)	1.3900
C(9)-C(14)	1.3900
C(10)-C(11)	1.3900
C(11)-C(12)	1.3900
C(12)-C(13)	1.3900
C(13)-C(14)	1.3900
C(14)-C(15)	1.522(3)
C(16)-C(18)	1.537(4)
C(16)-C(17)	1.536(4)
C(16)-C(19)	1.542(4)
C(19)-C(20)	1.531(4)
C(20)-C(21)	1.520(4)
C(21)-C(22)	1.519(3)
C(22)-C(23)	1.526(3)
C(22)-C(24)	1.545(3)
O(1)-N(1)-C(22)	106.28(17)
O(1)-N(1)-C(16)	106.84(18)
C(22)-N(1)-C(16)	117.46(19)
C(15)-O(1)-N(1)	112.22(17)
C(2)-C(1)-C(6)	120.0
C(3)-C(2)-C(1)	120.0
C(4)-C(3)-C(2)	120.0
C(3)-C(4)-C(5)	120.0
C(6)-C(5)-C(4)	120.0
C(5)-C(6)-C(1)	120.0
C(5)-C(6)-C(7)	118.7(2)
C(1)-C(6)-C(7)	121.2(2)
C(6)-C(7)-C(8)	113.2(2)
C(7)-C(8)-C(15)	113.2(2)
C(10)-C(9)-C(14)	120.0
C(9)-C(10)-C(11)	120.0
C(10)-C(11)-C(12)	120.0
C(13)-C(12)-C(11)	120.0
C(12)-C(13)-C(14)	120.0
C(13)-C(14)-C(9)	120.0
C(13)-C(14)-C(15)	120.92(17)
C(9)-C(14)-C(15)	119.07(17)
O(1)-C(15)-C(14)	113.90(18)
O(1)-C(15)-C(8)	103.3(2)
C(14)-C(15)-C(8)	113.68(19)
N(1)-C(16)-C(18)	116.0(2)
N(1)-C(16)-C(17)	108.5(2)

C(18)-C(16)-C(17)	106.0(2)
C(18)-C(16)-C(19)	111.0(2)
C(17)-C(16)-C(19)	106.9(2)
C(20)-C(19)-C(16)	112.8(2)
C(21)-C(20)-C(19)	108.6(2)
C(20)-C(21)-C(22)	113.2(2)
N(1)-C(22)-C(21)	107.9(2)
N(1)-C(22)-C(23)	108.0(2)
C(21)-C(22)-C(23)	108.3(2)
N(1)-C(22)-C(24)	115.5(2)
C(21)-C(22)-C(24)	110.0(2)
C(23)-C(22)-C(24)	106.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A 2 x 10 3) for ts002.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	37(1)	30(1)	43(1)	5(1)	-1(1)	-6(1)
O(1)	39(1)	42(1)	40(1)	-3(1)	-2(1)	-4(1)
C(1)	57(2)	74(2)	62(2)	-17(2)	-4(2)	-5(2)
C(2)	96(3)	101(3)	53(3)	-12(2)	8(2)	-22(3)
C(3)	134(4)	61(2)	55(3)	9(2)	-24(3)	-34(2)
C(4)	91(3)	48(2)	81(3)	4(2)	-34(2)	3(2)
C(5)	51(2)	47(2)	59(2)	0(2)	-11(2)	2(2)
C(6)	40(2)	36(2)	49(2)	-3(1)	-12(2)	-7(1)
C(7)	47(2)	42(2)	67(2)	4(2)	-15(2)	-8(1)
C(8)	36(2)	50(2)	50(2)	2(1)	-8(2)	-3(1)
C(9)	41(2)	51(2)	47(2)	-8(2)	-2(2)	-9(2)
C(10)	35(2)	67(2)	70(2)	-27(2)	-4(2)	-3(2)
C(11)	49(2)	40(2)	83(3)	-14(2)	-26(2)	4(2)
C(12)	51(2)	42(2)	66(2)	4(2)	-10(2)	-2(2)
C(13)	38(2)	45(2)	44(2)	-1(2)	-5(1)	-5(1)
C(14)	31(2)	39(2)	38(2)	-3(1)	-8(1)	-6(1)
C(15)	40(2)	36(1)	38(2)	-3(1)	-8(1)	-5(1)
C(16)	57(2)	32(2)	47(2)	-2(1)	-4(2)	4(1)
C(17)	96(3)	43(2)	56(2)	6(2)	-23(2)	12(2)
C(18)	81(2)	53(2)	67(2)	0(2)	-3(2)	27(2)
C(19)	88(3)	34(2)	66(2)	5(2)	9(2)	-12(2)
C(20)	76(3)	48(2)	77(3)	3(2)	-1(2)	-18(2)
C(21)	50(2)	43(2)	72(2)	-4(2)	-6(2)	-9(2)
C(22)	37(2)	38(2)	43(2)	-3(1)	-3(1)	-5(1)
C(23)	40(2)	44(2)	57(2)	0(1)	-14(1)	-1(1)
C(24)	57(2)	54(2)	50(2)	-8(2)	-13(2)	0(2)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ts002.

	x	y	z	U(eq)
H(1A)	6022	9988	2538	77
H(2A)	6586	8978	3416	100
H(3A)	8887	7758	3495	101
H(4A)	10624	7548	2696	89
H(5A)	10060	8558	1819	63
H(7A)	8693	10266	1355	63
H(7B)	6973	10698	1592	63
H(8A)	7274	8488	1031	55
H(8B)	6815	9620	660	55
H(9A)	2679	9905	1909	55
H(10A)	1064	11587	1862	69
H(11A)	1291	12865	1067	70
H(12A)	3133	12462	320	64
H(13A)	4748	10780	367	51
H(15A)	4810	8737	1581	46
H(17A)	5552	7031	1672	98
H(17B)	4904	5829	1921	98
H(17C)	3888	6989	2026	98
H(18A)	5630	6172	644	101
H(18B)	4063	5486	390	101
H(18C)	5095	4983	940	101
H(19A)	2410	4860	1454	75
H(19B)	1500	6009	1656	75
H(20A)	1323	5099	477	80
H(20B)	-157	5068	925	80
H(21A)	-319	7104	920	66
H(21B)	-486	6653	259	66
H(23A)	290	8743	7	71
H(23B)	1996	9248	257	71
H(23C)	537	8995	693	71
H(24A)	2818	6293	-122	81
H(24B)	3325	7593	-269	81
H(24C)	1551	7121	-466	81