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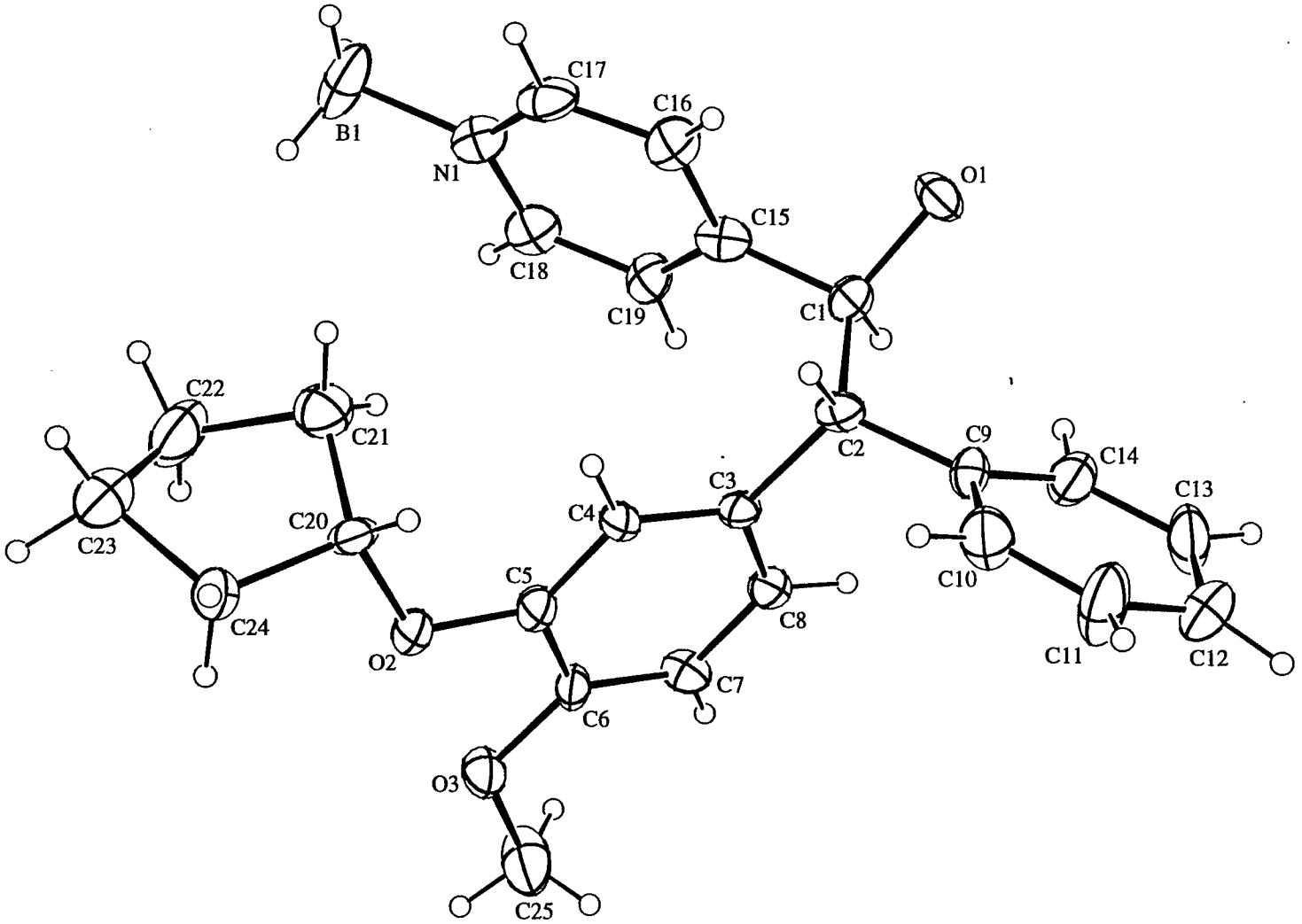

ORTEP drawing of compound 13 showing the crystallographic numbering scheme. Ellipsoids are drawn at a 20% probablity envelope except for the H atoms which are an arbitrary size.The methanol and water solvate molecules have been omitted.

Table of Selected Interatomic Distances[a]

Atom1	Atom2	Distance	Atom1	Atom2	Distance	Atom1	Atom2	Distance
O1	C1	1.45 (2)	C3	C4	1.37 (2)	C15	C16	1.40 (2)
O2	C5	1.37 (2)	C3	C8	1.39 (2)	C15	C19	1.36 (2)
O2	C20	1.47 (1)	C4	C5	1.35 (2)	C16	C17	1.41 (2)
O3	C6	1.40 (1)	C5	C6	1.41 (2)	C18	C19	1.39 (2)
O3	C25	1.44 (2)	C6	C7	1.37 (2)	C20	C21	1.50 (2)
N1	C17	1.35 (2)	C7	C8	1.37 (2)	C20	C24	1.53 (2)
N1	C18	1.35 (2)	C9	C10	1.36 (2)	C21	C22	1.57 (2)
N1	B1	1.59 (2)	C9	C14	1.39 (2)	C22	C23	1.46 (3)
C1	C2	1.55 (2)	C10	C11	1.34 (2)	C23	C24	1.55 (2)
C1	C15	1.51 (2)	C11	C12	1.42 (3)	C100	O101	1.47 (3)
C2	C3	1.52 (2)	C12	C13	1.33 (2)			
C2	C9	1.50 (2)	C13	C14	1.37 (2)			

[a]In angstroms. Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Selected Interatomic Angles[a]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C5	O2	C20	117 (1)	O2	C5	C4	126 (1)	C9	C14	C13	121 (2)
C6	O3	C25	116 (1)	O2	C5	C6	114 (1)	C1	C15	C16	120 (2)
C17	N1	C18	115 (2)	C4	C5	C6	120 (1)	C1	C15	C19	123 (2)
C17	N1	B1	120 (2)	O3	C6	C5	116 (1)	C16	C15	C19	117 (2)
C18	N1	B1	125 (2)	O3	C6	C7	125 (1)	C15	C16	C17	118 (2)
O1	C1	C2	111 (1)	C5	C6	C7	119 (1)	N1	C17	C16	125 (2)
O1	C1	C15	109 (1)	C6	C7	C8	119 (1)	N1	C18	C19	124 (2)
C2	C1	C15	110 (1)	C3	C8	C7	121 (1)	C15	C19	C18	121 (2)
C1	C2	C3	111 (1)	C2	C9	C10	120 (2)	O2	C20	C21	110 (1)
C1	C2	C9	114 (1)	C2	C9	C14	123 (2)	O2	C20	C24	106 (1)
C3	C2	C9	114 (1)	C10	C9	C14	117 (2)	C21	C20	C24	106 (1)
C2	C3	C4	122 (1)	C9	C10	C11	123 (2)	C20	C21	C22	102 (1)
C2	C3	C8	119 (1)	C10	C11	C12	119 (2)	C21	C22	C23	108 (2)
C4	C3	C8	119 (1)	C11	C12	C13	118 (2)	C22	C23	C24	101 (2)
C3	C4	C5	121 (1)	C12	C13	C14	121 (2)	C20	C24	C23	108 (1)

[a]In degrees. Numbers in parentheses are estimated standard deviations in the least significant digits.

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Table of Positional and Thermal Parameters and Their Estimated Standard Deviations.

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	-224.0(8)	408.8(3)	186.2(8)	8.8(6)	4.3(5)	7.6(6)	1.1(5)	-0.5(6)	-1.2(5)
O2	18.0(8)	136.9(3)	138.3(7)	10.4(7)	5.4(5)	4.2(5)	1.0(6)	0.2(6)	0.8(4)
O3	-72.5(8)	111.9(3)	-87.4(7)	10.0(7)	5.2(5)	5.6(5)	0.3(5)	-1.3(6)	-0.2(5)
O4	-386.9(9)	469.4(4)	37.4(9)	10.6(8)	8.3(6)	10.2(8)	0.4(7)	-1.9(8)	-2.1(7)
N1	-340.0(9)	235.7(4)	432.1(9)	5.8(7)	9.1(8)	6.0(7)	0.0(7)	-0.1(7)	-0.6(7)
C1	-224(1)	352.9(5)	133(1)	7.2(9)	6.5(8)	4.5(7)	0.3(9)	-0.6(8)	0.4(8)
C2	-93(1)	335.5(4)	89(1)	3.5(7)	6.6(8)	4.9(7)	1.4(7)	0.2(7)	-0.2(7)
C3	-92(1)	275.3(4)	44(1)	6.5(8)	4.4(7)	3.5(6)	-0.8(7)	0.4(7)	-0.9(6)
C4	-39(1)	234.1(4)	118(1)	6.9(9)	4.2(6)	4.2(7)	0.7(8)	-0.1(8)	-0.5(6)
C5	-35(1)	181.1(5)	75(1)	10(1)	5.4(7)	4.1(7)	0.8(9)	-0.4(9)	0.6(7)
C6	-84(1)	167.6(4)	-50(1)	6.6(9)	4.1(7)	5.1(7)	-0.4(7)	0.1(8)	1.2(6)
C7	-141(1)	207.9(5)	-122(1)	5.7(8)	6.2(8)	5.5(8)	0.2(8)	-1.4(8)	-1.4(7)
C8	-142(1)	261.7(5)	-77(1)	6.9(9)	6.0(8)	4.7(7)	1.3(8)	0.0(9)	0.2(8)
C9	-33(1)	375.2(4)	-5(1)	5.7(8)	5.2(7)	4.5(7)	-0.3(8)	-1.1(8)	1.1(7)
C10	92(1)	377.9(5)	-12(1)	8(1)	7.3(9)	10(1)	0(1)	0(1)	1(1)
C11	152(1)	410.0(6)	-98(2)	9(1)	11(1)	16(1)	-2(1)	3(1)	7(1)
C12	84(1)	439.9(6)	-193(1)	12(1)	10(1)	9(1)	-1(1)	5(1)	3(1)
C13	-38(1)	440.8(5)	-182(1)	10(1)	6.2(8)	13(1)	1(1)	1(1)	4.3(9)
C14	-98(1)	406.6(5)	-96(1)	8(1)	9(1)	7.4(9)	1(1)	2(1)	2.5(9)
C15	-270(1)	313.7(5)	237(1)	4.4(8)	7.8(9)	5.9(9)	0.5(8)	-0.9(8)	-1.7(8)
C16	-233(1)	320.3(6)	367(1)	11(1)	8(1)	6.6(9)	0(1)	0(1)	0.2(9)
C17	-268(1)	279.7(6)	459(1)	9(1)	12(1)	3.8(8)	5(1)	-1.3(9)	-0.9(9)

Table of Positional and Thermal Parameters and Their Estimated Standard Deviations (continued).

Atom	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C18	-373(1)	230.6(5)	305(1)	4.2(9)	9(1)	8(1)	0.2(9)	0.7(9)	0(1)
C19	-341(1)	268.3(5)	208(1)	6.3(9)	7.6(9)	5.6(8)	0.6(9)	-1.3(9)	0.8(8)
C20	54(1)	145.5(5)	276(1)	6.2(9)	8.1(9)	3.4(7)	1.7(9)	0.9(8)	0.0(7)
C21	-59(1)	148.2(6)	360(1)	10(1)	10(1)	6.7(9)	2(1)	-1(1)	-0.7(9)
C22	-73(2)	86.4(6)	406(1)	14(1)	12(1)	8(1)	-2(1)	2(1)	3(1)
C23	51(2)	64.6(6)	430(1)	14(1)	13(1)	9(1)	3(1)	3(1)	3(1)
C24	124(1)	93.2(5)	318(1)	12(1)	9(1)	6.0(9)	4(1)	1(1)	1.9(9)
C25	-106(2)	99.3(5)	-221(1)	21(2)	7(1)	7(1)	1(1)	-4(1)	-0.4(9)
B1	-378(2)	193.3(8)	545(2)	9(2)	17(2)	10(1)	0(2)	2(1)	8(1)

Atom	x	y	z	U	Atom	x	y	z	U
O101	426(2)	31.9(6)	588(2)	26.5(8)	C100	558(2)	36.2(8)	615(2)	18.1(9)

The atomic positional parameters have been multiplied by 10^3.
The anisotropic thermal parameters have been multiplied by 10^2.
The isotropic thermal parameters have been multiplied by 10^2.
The form of the anisotropic thermal parameter is $\exp[-2\pi^2(h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23})]$
Estimated standard deviations in the least significant digits are shown in parentheses.

Table of Derived Positional and Thermal Parameters for Hydrogen Atoms.

Atom	x	y	z	U, Å^2	Atom	x	y	z	U, Å^2
HC1	-270	351	57	8	H1C21	-125	159	314	9
HC2	-39	338	165	6	H2C21	-43	171	436	9
HC4	-8	241	199	5	H1C22	-104	66	339	12
HC7	-179	199	-198	6	H2C22	-116	85	485	12
HC8	-173	289	-128	6	H1C23	57	21	424	13
HC10	131	358	44	10	H2C23	83	70	518	13
HC11	232	415	-94	13	H1C24	201	105	352	11
HC12	125	458	-257	13	H2C24	131	70	248	11
HC13	-86	462	-233	10	H1C25	-97	62	-230	14
HC14	-183	408	-86	9	H2C25	-191	110	-227	14
HC16	-180	345	390	10	H3C25	-57	121	-272	14
HC17	-243	285	544	9	H1B1	-346	208	624	12
HC18	-416	202	288	8	H2B1	-462	191	550	14
HC19	-365	262	123	7	H3B1	-341	158	522	14
HC20	99	177	284	7					

The positional and thermal parameters have been multiplied by 10^3 and 10^2 respectively.