Table of experimental details

Compound ID	**13**	**16**
Formula	$C_{37}H_{38}N_2O_6$	$C_{28}H_{28}FN_3O$
Fw	606.725	441.553
Crystal colour	colourless	colourless
Crystal dimen. (mm)	0.04 x 0.09 x 0.30	0.05 x 0.10 x 0.38
Lattice symmetry	monoclinic	monoclinic
Space group	$P2_1$	$C2$
a , (Å)	11.226(1)	20.678(2)
b	11.081(1)	6.033(3)
c	13.191(1)	18.118(2)
α	90	90
β	95.173(7)	96.506(7)
γ	90	90
V (Å^3)	1634.2(5)	2246(2)
Z	2	4
D_{calc} (Mg m^{-3})	1.233	1.306
Radiation ($K\alpha$)	Cu	Cu
Wavelength (Å)	1.541838	1.541838
Temperature (K)	294	294
μ (mm^{-1})	0.64	0.65
Diffractometer	Rigaku AFC5	Rigaku AFC5
Reflections measured	3431	2482
Resolution (Å)	0.81	0.81
Unique reflections	3265	2413
R_{int}	0.036	0.021
Absorp. corr.	none	none
Trans. (max, min)		
Reflections used	3264	2413
Refl. obsd. criterion	$> 2\sigma(I)$	$> 2\sigma(I)$
Variables	406	298
Refined on	F^2	F^2
R	0.051	0.042
R_w	0.114	0.123
S	1.15	1.05
residual peak (eÅ^{-3})	0.19(5)	0.16(4)
Computer programs:		
Solution	SHELXS-86	SHELXS-86
Refinement	SHELXL-93	SHELXL-93

Table of atomic parameters for compound **13**
Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)

$$Ueq = (1/3)S_i S_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	*y*	*z*	*Ueq*
O8	0.5449(4)	1.1185(6)	0.5143(4)	0.071(2)
O9	0.5827(4)	1.2151(5)	0.3695(4)	0.067(2)
O17	0.9484(3)	1.0234(4)	0.6723(3)	0.0477(12)
O19	0.8809(5)	1.1363(5)	0.7980(4)	0.083(2)
O21	0.9731(4)	0.8359(4)	0.7988(3)	0.0534(13)
O29	1.0600(6)	0.6581(6)	0.8412(4)	0.089(2)
N1	0.7311(5)	1.1288(7)	0.4637(4)	0.059(2)
N33	1.3109(4)	1.1726(6)	0.5795(4)	0.054(2)
C2	0.7843(5)	1.0519(8)	0.5465(5)	0.057(2)
C3	0.8982(5)	1.1106(7)	0.5959(4)	0.047(2)
C4	0.9876(6)	1.1306(7)	0.5173(5)	0.048(2)
C5	0.9262(5)	1.2197(8)	0.4396(5)	0.058(2)
C6	0.8137(5)	1.1622(8)	0.3878(5)	0.064(2)
C7	0.6142(6)	1.1507(8)	0.4538(5)	0.055(2)
C10	0.4570(7)	1.2450(12)	0.3522(7)	0.111(4)
C11	0.4423(7)	1.3166(13)	0.2550(7)	0.080(3)
C12	0.4517(9)	1.4419(14)	0.2588(8)	0.099(3)
C13	0.4398(10)	1.5110(13)	0.1699(12)	0.125(4)
C14	0.4192(11)	1.4500(17)	0.0787(10)	0.123(5)
C15	0.4077(11)	1.3297(17)	0.0720(9)	0.125(5)
C16	0.4222(9)	1.2615(13)	0.1630(9)	0.117(4)
C18	0.9326(6)	1.0494(8)	0.7697(5)	0.053(2)
C20	0.9885(6)	0.9576(7)	0.8419(4)	0.043(2)
C22	1.0564(7)	0.7643(8)	0.8530(5)	0.058(2)
C23	1.1237(6)	0.8444(7)	0.9306(5)	0.052(2)
C24	1.0328(7)	0.8710(7)	1.0083(5)	0.060(2)
C25	0.9372(7)	0.9499(8)	0.9452(5)	0.064(2)
C26	1.1275(6)	0.9627(7)	0.8692(5)	0.051(2)
C27	1.1663(8)	1.0747(7)	0.9301(7)	0.080(3)
C28	1.1978(6)	0.9531(9)	0.7756(6)	0.070(2)
C30	1.2418(7)	0.7908(9)	0.9750(6)	0.086(3)
C31	1.1108(5)	1.1695(7)	0.5595(5)	0.044(2)
C32	1.2138(5)	1.1237(7)	0.5241(4)	0.046(2)
C34	1.2737(6)	1.2526(8)	0.6519(5)	0.055(2)
C35	1.3390(8)	1.3235(9)	0.7208(6)	0.073(2)
C36	1.2781(10)	1.3946(9)	0.7836(6)	0.083(3)
C37	1.1536(10)	1.3942(8)	0.7755(7)	0.082(3)
C38	1.0873(8)	1.3260(7)	0.7046(6)	0.068(2)
C39	1.1467(6)	1.2513(6)	0.6399(5)	0.047(2)
C40	1.2320(6)	1.0426(8)	0.4383(5)	0.051(2)
C41	1.1786(6)	1.0668(9)	0.3423(5)	0.067(3)
C42	1.1995(8)	0.9946(11)	0.2617(6)	0.085(3)
C43	1.2747(10)	0.8967(11)	0.2750(8)	0.095(4)
C44	1.3283(9)	0.8725(10)	0.3689(8)	0.097(3)
C45	1.3064(7)	0.9453(9)	0.4516(6)	0.069(2)

Table of atomic parameters for compound **13**(continues)

	x	*y*	*z*	*Ueq*
H33	1.3985(4)	1.1486(6)	0.5778(4)	0.065
H2A	0.8030(5)	0.9733(8)	0.5197(5)	0.068
H2B	0.7276(5)	1.0407(8)	0.5970(5)	0.068
H3	0.8796(5)	1.1870(7)	0.6283(4)	0.057
H4	0.9962(6)	1.0537(7)	0.4820(5)	0.058
H5A	0.9057(5)	1.2932(8)	0.4739(5)	0.070
H5B	0.9805(5)	1.2404(8)	0.3890(5)	0.070
H6A	0.7747(5)	1.2186(8)	0.3393(5)	0.076
H6B	0.8350(5)	1.0908(8)	0.3509(5)	0.076
H10A	0.4320(7)	1.2924(12)	0.4084(7)	0.133
H10B	0.4091(7)	1.1721(12)	0.3459(7)	0.133
H12	0.4660(9)	1.4801(14)	0.3215(8)	0.119
H13	0.4457(10)	1.5947(13)	0.1720(12)	0.150
H14	0.4128(11)	1.4948(17)	0.0188(10)	0.148
H15	0.3908(11)	1.2922(17)	0.0093(9)	0.151
H16	0.4180(9)	1.1778(13)	0.1597(9)	0.140
H24A	1.0696(7)	0.9150(7)	1.0665(5)	0.072
H24B	0.9978(7)	0.7971(7)	1.0317(5)	0.072
H25A	0.8594(7)	0.9112(8)	0.9395(5)	0.077
H25B	0.9304(7)	1.0292(8)	0.9753(5)	0.077
H27A	1.1219(8)	1.0802(7)	0.9888(7)	0.120
H27B	1.1514(8)	1.1450(7)	0.8884(7)	0.120
H27C	1.2502(8)	1.0695(7)	0.9515(7)	0.120
H28A	1.1729(6)	0.8823(9)	0.7375(6)	0.105
H28B	1.2817(6)	0.9477(9)	0.7968(6)	0.105
H28C	1.1829(6)	1.0233(9)	0.7337(6)	0.105
H30A	1.2802(7)	0.8459(9)	1.0237(6)	0.129
H30B	1.2925(7)	0.7771(9)	0.9213(6)	0.129
H30C	1.2271(7)	0.7157(9)	1.0079(6)	0.129
H35	1.4222(8)	1.3237(9)	0.7249(6)	0.088
H36	1.3202(10)	1.4433(9)	0.8319(6)	0.100
H37	1.1140(10)	1.4419(8)	0.8198(7)	0.099
H38	1.0042(8)	1.3292(7)	0.6994(6)	0.081
H41	1.1278(6)	1.1329(9)	0.3322(5)	0.081
H42	1.1625(8)	1.0118(11)	0.1974(6)	0.102
H43	1.2886(10)	0.8477(11)	0.2200(8)	0.114
H44	1.3799(9)	0.8070(10)	0.3784(8)	0.116
H45	1.3427(7)	0.9275(9)	0.5161(6)	0.083

Table of atomic parameters for compound **16**
Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)

$$Ueq = (1/3)\mathrm{S}_i\,\mathrm{S}_j\,U_{ij}\,a_i^*a_j^*\,\mathbf{a}_i\bullet\mathbf{a}_j$$

	x	*y*	*z*	*Ueq*
F18	0.0413(1)	0.1128(5)	0.0855(2)	0.07814(8)
O9	0.2496(1)	-0.4736(6)	0.2459(2)	0.06454(8)
N1	0.1465(1)	-0.3771(7)	0.2037(2)	0.05349(9)
N8	0.1686(1)	-0.6257(6)	0.3028(2)	0.04391(7)
N21	-0.1321(1)	-0.0709(5)	0.1885(2)	0.04197(7)
C2	0.0758(1)	-0.3862(7)	0.2050(2)	0.04471(9)
C3	0.0442(1)	-0.1629(6)	0.1784(2)	0.03931(8)
C4	0.0654(2)	-0.0985(7)	0.1037(2)	0.0492(1)
C5	0.1379(2)	-0.0915(9)	0.1064(2)	0.0667(2)
C6	0.1670(2)	-0.311(1)	0.1321(2)	0.0771(3)
C7	0.1906(2)	-0.4936(7)	0.2503(2)	0.0460(1)
C10	0.2161(2)	-0.7638(8)	0.3493(2)	0.0505(1)
C11	0.2445(3)	-0.940(1)	0.3036(3)	0.0978(5)
C12	0.1841(2)	-0.8567(7)	0.4141(2)	0.0444(1)
C13	0.1849(2)	-0.7353(9)	0.4794(2)	0.0627(2)
C14	0.1567(2)	-0.822(1)	0.5387(2)	0.0783(4)
C15	0.1272(2)	-1.025(1)	0.5333(3)	0.0894(5)
C16	0.1264(2)	-1.146(1)	0.4699(3)	0.0815(3)
C17	0.1548(2)	-1.0620(8)	0.4105(2)	0.0594(2)
C19	-0.0291(1)	-0.1693(6)	0.1756(2)	0.03957(8)
C20	-0.0674(1)	-0.0294(6)	0.2121(2)	0.03839(8)
C22	-0.1365(2)	-0.2403(7)	0.1384(2)	0.04263(9)
C23	-0.1917(2)	-0.3450(9)	0.1034(2)	0.0536(1)
C24	-0.1822(2)	-0.5241(9)	0.0590(2)	0.0646(2)
C25	-0.1197(2)	-0.5938(9)	0.0477(2)	0.0655(2)
C26	-0.0655(2)	-0.4866(8)	0.0809(2)	0.0532(1)
C27	-0.0724(2)	-0.3076(6)	0.1282(2)	0.04038(9)
C28	-0.0513(1)	0.1436(6)	0.2682(2)	0.03856(8)
C29	-0.0873(2)	0.3392(7)	0.2675(2)	0.0451(1)
C30	-0.0732(2)	0.4997(8)	0.3205(2)	0.0558(1)
C31	-0.0236(2)	0.4698(8)	0.3768(2)	0.0590(2)
C32	0.0120(2)	0.2766(9)	0.3797(2)	0.0583(2)
C33	-0.0012(2)	0.1144(8)	0.3264(2)	0.0502(1)

Table of atomic parameters for compound **16** (continued)

	x	*y*	*z*	*Ueq*
H2A	0.0660(1)	-0.4174(7)	0.2551(2)	0.053650
H2B	0.0577(1)	-0.5048(7)	0.1729(2)	0.053650
H3	0.0602(1)	-0.0489(6)	0.2145(2)	0.047170
H4	0.0477(2)	-0.2046(7)	0.0658(2)	0.058990
H5A	0.1551(2)	0.0245(9)	0.1402(2)	0.080030
H5B	0.1499(2)	-0.0574(9)	0.0574(2)	0.080030
H6A	0.1537(2)	-0.423(1)	0.0952(2)	0.092470
H6B	0.2141(2)	-0.300(1)	0.1366(2)	0.092470
H8	0.1203(1)	-0.6200(6)	0.2975(2)	0.052700
H10	0.2518(2)	-0.6671(8)	0.3697(2)	0.060550
H11A	0.2639(3)	-0.872(1)	0.2636(3)	0.146740
H11B	0.2107(3)	-1.039(1)	0.2836(3)	0.146740
H11C	0.2771(3)	-1.022(1)	0.3344(3)	0.146740
H13	0.2044(2)	-0.5961(9)	0.4832(2)	0.075260
H14	0.1577(2)	-0.741(1)	0.5826(2)	0.093930
H15	0.1076(2)	-1.080(1)	0.5732(3)	0.107240
H16	0.1067(2)	-1.285(1)	0.4667(3)	0.097740
H17	0.1542(2)	-1.1454(8)	0.3672(2)	0.071330
H21	-0.1596(1)	0.0138(5)	0.2097(2)	0.050370
H23	-0.2333(2)	-0.2957(9)	0.1099(2)	0.064290
H24	-0.2180(2)	-0.6004(9)	0.0361(2)	0.077570
H25	-0.1147(2)	-0.7149(9)	0.0171(2)	0.078560
H26	-0.0242(2)	-0.5332(8)	0.0719(2)	0.063860
H29	-0.1216(2)	0.3613(7)	0.2304(2)	0.054080
H30	-0.0974(2)	0.6299(8)	0.3183(2)	0.066990
H31	-0.0142(2)	0.5790(8)	0.4127(2)	0.070840
H32	0.0454(2)	0.2552(9)	0.4180(2)	0.069950
H33	0.0233(2)	-0.0153(8)	0.3291(2)	0.060290

Table of selected interatomic distances (Å) and angles for **13**

O8—C7	1.217(7)	C18—C20	1.492(10)
O9—C7	1.342(8)	C20—C25	1.528(8)
O9—C10	1.447(8)	C20—C26	1.571(9)
O17—C18	1.345(8)	C22—C23	1.506(10)
O17—C3	1.471(7)	C23—C30	1.520(10)
O19—C18	1.201(9)	C23—C24	1.538(9)
O21—C22	1.376(9)	C23—C26	1.543(10)
O21—C20	1.468(8)	C24—C25	1.565(10)
O29—C22	1.188(9)	C26—C27	1.521(10)
N1—C7	1.329(8)	C26—C28	1.528(9)
N1—C2	1.469(9)	C31—C32	1.382(8)
N1—C6	1.472(8)	C31—C39	1.426(9)
N33—C32	1.368(8)	C32—C40	1.474(10)
N33—C34	1.395(9)	C34—C35	1.364(10)
C2—C3	1.528(9)	C34—C39	1.420(9)
C3—C4	1.522(8)	C35—C36	1.370(11)
C4—C31	1.506(9)	C36—C37	1.393(12)
C4—C5	1.541(10)	C37—C38	1.370(11)
C5—C6	1.520(9)	C38—C39	1.400(9)
C10—C11	1.504(12)	C40—C45	1.366(11)
C11—C16	1.360(14)	C40—C41	1.379(9)
C11—C12	1.393(15)	C41—C42	1.368(11)
C12—C13	1.397(15)	C42—C43	1.376(13)
C13—C14	1.38(2)	C43—C44	1.354(13)
C14—C15	1.34(2)	C44—C45	1.397(11)
C15—C16	1.42(2)		

C7—O9—C10	115.7(6)	O21—C22—C23	106.8(7)
C18—O17—C3	116.0(6)	C22—C23—C30	113.4(7)
C22—O21—C20	106.2(5)	C22—C23—C24	104.1(6)
C7—N1—C2	120.6(6)	C30—C23—C24	115.2(6)
C7—N1—C6	124.4(6)	C22—C23—C26	100.4(6)
C2—N1—C6	114.4(5)	C30—C23—C26	118.0(6)
C32—N33—C34	110.1(5)	C24—C23—C26	103.8(6)
N1—C2—C3	109.8(6)	C23—C24—C25	102.5(5)
O17—C3—C4	109.1(5)	C20—C25—C24	102.1(6)
O17—C3—C2	105.4(6)	C27—C26—C28	109.8(7)
C4—C3—C2	110.5(5)	C27—C26—C23	115.8(6)
C31—C4—C3	115.5(5)	C28—C26—C23	114.0(7)
C31—C4—C5	113.8(6)	C27—C26—C20	112.5(6)
C3—C4—C5	105.3(5)	C28—C26—C20	112.8(6)
C6—C5—C4	109.5(7)	C23—C26—C20	90.9(5)
N1—C6—C5	110.4(5)	C32—C31—C39	107.2(6)
O8—C7—N1	124.5(6)	C32—C31—C4	122.6(6)
O8—C7—O9	124.2(6)	C39—C31—C4	130.2(6)
N1—C7—O9	111.2(6)	N33—C32—C31	109.0(6)
O9—C10—C11	106.7(6)	N33—C32—C40	119.5(5)
C16—C11—C12	119.1(11)	C31—C32—C40	131.4(6)
C16—C11—C10	121.4(13)	C35—C34—N33	130.2(7)

C12—C11—C10	119.5(11)	C35—C34—C39	123.7(8)
C11—C12—C13	121.0(11)	N33—C34—C39	106.1(6)
C14—C13—C12	117.4(14)	C34—C35—C36	117.8(8)

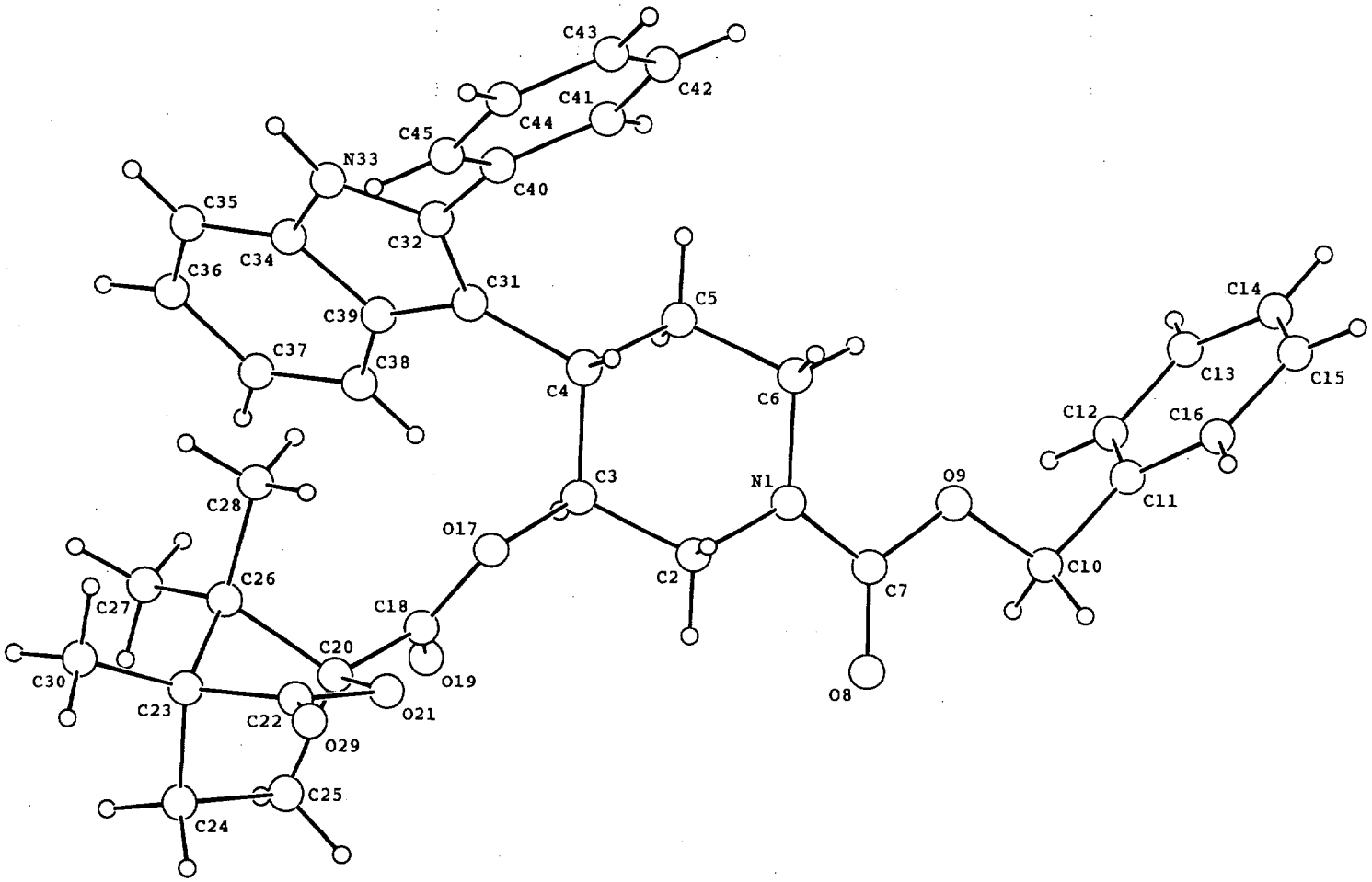
Table of selected interatomic distances (Å) and angles for **13** (continued)

C15—C14—C13	123.4(14)	C35—C36—C37	120.2(8)
C14—C15—C16	118.1(13)	C38—C37—C36	122.3(8)
C11—C16—C15	121.0(14)	C37—C38—C39	118.9(8)
O19—C18—O17	125.3(7)	C38—C39—C34	117.0(7)
O19—C18—C20	122.3(7)	C38—C39—C31	135.3(7)
O17—C18—C20	112.4(7)	C34—C39—C31	107.6(6)
O21—C20—C18	110.6(5)	C45—C40—C41	118.8(7)
O21—C20—C25	104.7(6)	C45—C40—C32	120.5(6)
C18—C20—C25	115.9(6)	C41—C40—C32	120.6(7)
O21—C20—C26	101.6(5)	C42—C41—C40	120.6(8)
C18—C20—C26	118.2(6)	C41—C42—C43	120.6(9)
C25—C20—C26	104.1(5)	C44—C43—C42	119.3(10)
O29—C22—O21	122.1(8)	C43—C44—C45	120.4(10)
O29—C22—C23	130.7(8)	C40—C45—C44	120.3(8)

Table of selected interatomic distances (Å) and angles for **16**

F18—C4	1.395(5)	C14—C15	1.37(1)
O9—C7	1.238(4)	C15—C16	1.361(9)
N1—C7	1.365(4)	C16—C17	1.382(7)
N1—C6	1.466(5)	C19—C20	1.376(5)
N1—C2	1.467(4)	C19—C27	1.435(5)
N8—C7	1.358(5)	C20—C28	1.470(5)
N8—C10	1.476(4)	C22—C23	1.393(5)
N21—C22	1.364(5)	C22—C27	1.418(4)
N21—C20	1.381(4)	C23—C24	1.375(7)
C2—C3	1.550(5)	C24—C25	1.396(6)
C3—C19	1.511(4)	C25—C26	1.372(6)
C3—C4	1.520(5)	C26—C27	1.396(6)
C4—C5	1.496(5)	C28—C29	1.395(5)
C5—C6	1.505(7)	C28—C33	1.403(5)
C10—C11	1.508(6)	C29—C30	1.371(6)
C10—C12	1.518(5)	C30—C31	1.374(6)
C12—C17	1.377(6)	C31—C32	1.376(7)
C12—C13	1.390(6)	C32—C33	1.380(6)
C13—C14	1.383(7)		

C7—N1—C6	116.6(3)	C15—C16—C17	119.6(5)
C7—N1—C2	124.7(3)	C12—C17—C16	121.2(5)
C6—N1—C2	114.4(3)	C20—C19—C27	106.9(3)
C7—N8—C10	118.5(3)	C20—C19—C3	126.7(3)
C22—N21—C20	109.2(3)	C27—C19—C3	126.1(3)
N1—C2—C3	110.4(3)	C19—C20—N21	109.3(3)
C19—C3—C4	111.5(3)	C19—C20—C28	132.1(3)
C19—C3—C2	112.0(3)	N21—C20—C28	118.6(3)
C4—C3—C2	110.2(3)	N21—C22—C23	129.1(3)
F18—C4—C5	108.2(4)	N21—C22—C27	108.0(3)
F18—C4—C3	108.2(3)	C23—C22—C27	122.8(4)
C5—C4—C3	111.6(3)	C24—C23—C22	117.2(4)
C4—C5—C6	110.4(4)	C23—C24—C25	121.3(4)
N1—C6—C5	111.6(4)	C26—C25—C24	121.1(5)
O9—C7—N8	120.8(3)	C25—C26—C27	119.9(4)
O9—C7—N1	120.3(4)	C26—C27—C22	117.6(3)
N8—C7—N1	118.8(3)	C26—C27—C19	135.8(3)
N8—C10—C11	111.2(3)	C22—C27—C19	106.5(3)
N8—C10—C12	109.3(3)	C29—C28—C33	117.5(4)
C11—C10—C12	113.3(4)	C29—C28—C20	121.0(3)
C17—C12—C13	118.5(4)	C33—C28—C20	121.5(3)
C17—C12—C10	121.5(4)	C30—C29—C28	121.3(3)
C13—C12—C10	120.0(4)	C29—C30—C31	120.6(4)
C14—C13—C12	119.8(5)	C30—C31—C32	119.4(4)
C15—C14—C13	120.5(5)	C31—C32—C33	120.8(4)
C16—C15—C14	120.4(5)	C32—C33—C28	120.5(4)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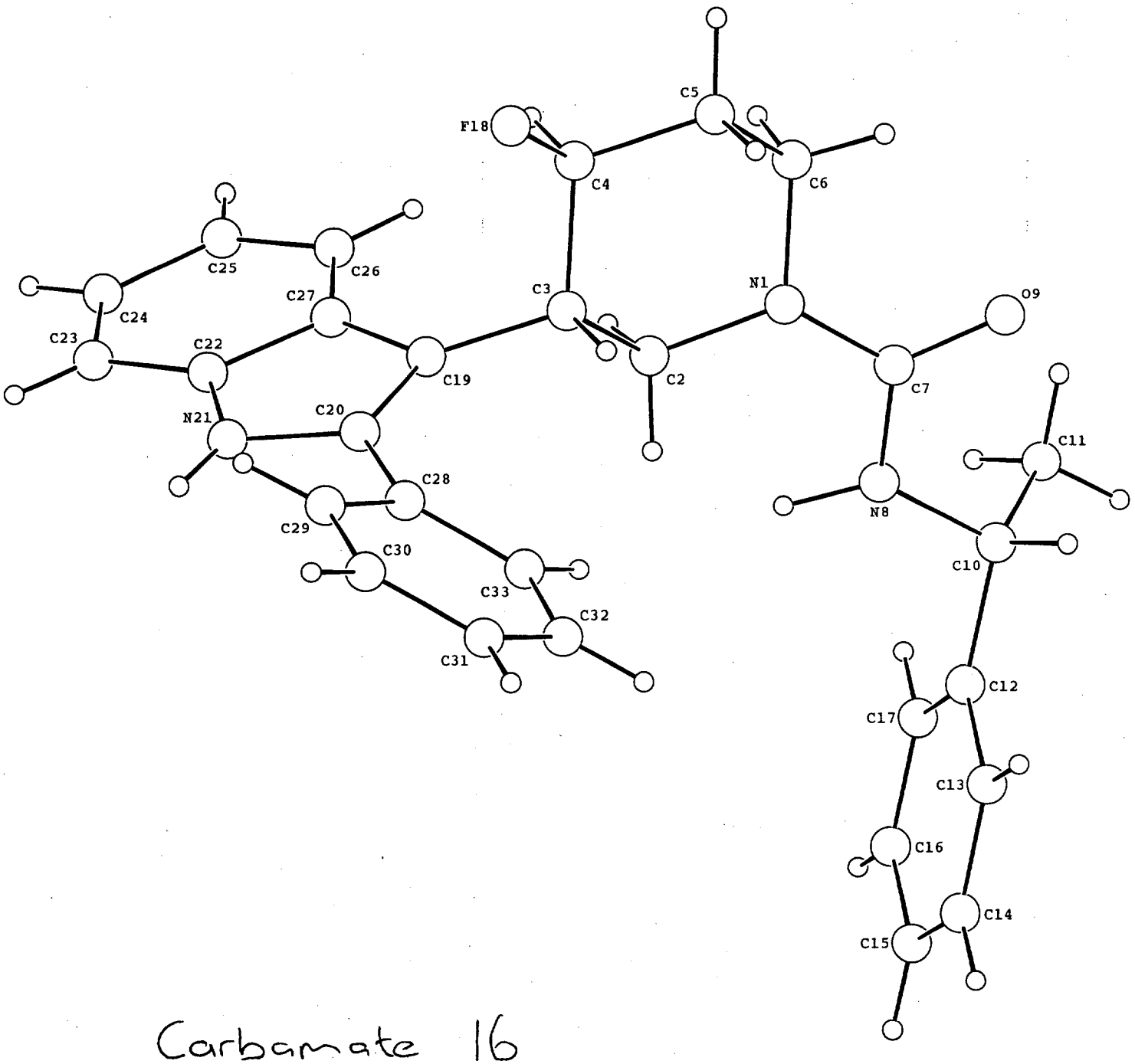

Carbamate 16