Table 1. Crystal data and structure refinement for N,N'-BIS(P-METOXYPHENYL)-FORMAMMIDINE

Empirical formula	C15 H16 N2 O2
Formula weight	256.30
Temperature	293(2) K
Wavelength	1.54178 A
Crystal system	TRICLINIC
Space group	P-1
Unit cell dimensions	a = 9.925(2) A alpha = 93.12(3) deg. b = 10.232(2) A beta = 106.80(3) deg. c = 14.980(3) A gamma = 107.76(3) deg.
Volume	1369.9(5) A^3
Z	4
Density (calculated)	1.243 Mg/m^3
Absorption coefficient	0.675 mm^-1
F(000)	544
Crystal size	0.3 x 0.3 x 0.25 mm
Theta range for data collection	3.12 to 80.24 deg.
Index ranges	-10<=h<=10, -11<=k<=11, 0<=l<=15
Reflections collected	5358
Independent reflections	5158 [R(int) = 0.0688]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5148 / 0 / 398
Goodness-of-fit on F^2	0.990
Final R indices [I>2sigma(I)]	R1 = 0.0544, wR2 = 0.1555
R indices (all data)	R1 = 0.0658, wR2 = 0.1850
Extinction coefficient	0.028(2)
Largest diff. peak and hole	0.249 and -0.256 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for N,N'-BIS(P-METOXYPHENYL)-FORMAMMIDINE
U(eq) is defined
as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(11)	4219(2)	7868(1)	3565(1)	53(1)
N(21)	3787(2)	8017(2)	5005(1)	54(1)
O(11)	432(2)	9249(1)	7127(1)	70(1)
O(21)	2644(2)	8946(2)	-137(1)	79(1)
C(11)	3505(2)	8174(2)	4112(1)	50(1)
C(21)	2962(2)	8398(1)	5539(1)	46(1)
C(31)	2484(2)	9540(1)	5413(1)	48(1)
C(41)	1621(2)	9850(1)	5918(1)	48(1)
C(51)	1264(2)	9037(2)	6581(1)	48(1)
C(61)	1775(2)	7925(2)	6735(1)	55(1)
C(71)	2608(2)	7606(2)	6216(1)	52(1)
C(81)	3775(2)	8064(1)	2612(1)	47(1)
C(91)	2278(2)	7706(2)	2071(1)	55(1)
C(101)	1859(2)	7982(2)	1155(1)	61(1)
C(111)	2937(2)	8602(2)	755(1)	57(1)
C(121)	4439(2)	8915(2)	1275(1)	62(1)
C(131)	4843(2)	8643(2)	2185(1)	57(1)
C(141)	6(3)	10437(3)	7078(2)	80(1)
C(151)	1162(3)	8875(4)	-612(2)	103(1)
N(12)	6411(2)	7189(2)	5950(1)	60(1)
N(22)	6737(2)	6793(2)	4521(1)	58(1)
O(12)	9480(2)	4990(1)	2173(1)	70(1)
O(22)	7092(3)	6585(2)	9712(1)	118(1)
C(12)	7082(2)	6746(2)	5429(1)	57(1)
C(22)	7453(2)	6344(1)	3941(1)	51(1)
C(32)	8935(2)	6379(2)	4270(1)	56(1)
C(42)	9566(2)	5919(2)	3661(1)	57(1)
C(52)	8753(2)	5436(2)	2718(1)	55(1)
C(62)	7293(2)	5411(2)	2384(1)	60(1)
C(72)	6661(2)	5870(2)	2997(1)	59(1)
C(82)	6673(2)	7051(2)	6909(1)	53(1)
C(92)	7185(2)	6034(2)	7327(1)	61(1)
C(102)	7324(2)	5915(2)	8256(1)	70(1)
C(112)	6943(2)	6793(2)	8797(1)	71(1)
C(122)	6442(2)	7814(2)	8394(1)	71(1)
C(132)	6318(2)	7931(2)	7467(1)	63(1)
C(142)	8743(3)	4612(3)	1198(2)	95(1)
C(152)	6369(6)	7225(4)	10204(2)	133(1)

Table 4. Bond lengths [A], angles [deg] and torsion angles [deg] for N,N'-BIS(P-METOXYPHENYL)-FORMAMMIDINE

N(11)-C(11)	1.308(2)
N(11)-C(81)	1.413(2)
N(11)-H(11)	0.78(5)
N(21)-C(11)	1.315(2)
N(21)-C(21)	1.415(2)
N(21)-H(21)	0.84(3)
O(11)-C(51)	1.370(2)
O(11)-C(141)	1.402(2)
O(21)-C(111)	1.372(2)
O(21)-C(151)	1.414(3)
C(11)-H(111)	0.99(2)
C(21)-C(71)	1.389(2)
C(21)-C(31)	1.391(2)
C(31)-C(41)	1.385(2)
C(31)-H(31)	0.93
C(41)-C(51)	1.385(2)
C(41)-H(41)	0.93
C(51)-C(61)	1.385(2)
C(61)-C(71)	1.379(2)
C(61)-H(61)	0.93
C(71)-H(71)	0.93
C(81)-C(131)	1.390(2)
C(81)-C(91)	1.392(2)
C(91)-C(101)	1.385(2)
C(91)-H(91)	0.93
C(101)-C(111)	1.380(3)
C(101)-H(101)	0.93
C(111)-C(121)	1.393(2)
C(121)-C(131)	1.374(2)
C(121)-H(121)	0.93
C(131)-H(131)	0.93
C(141)-H(143)	0.96
C(141)-H(144)	0.96
C(141)-H(145)	0.96
C(151)-H(153)	0.96
C(151)-H(154)	0.96
C(151)-H(155)	0.96
N(12)-C(12)	1.306(2)
N(12)-C(82)	1.406(2)
N(12)-H(12)	0.84(5)
N(22)-C(12)	1.311(2)
N(22)-C(22)	1.409(2)
N(22)-H(22)	0.89(4)
O(12)-C(52)	1.377(2)
O(12)-C(142)	1.403(3)
O(22)-C(112)	1.370(2)
O(22)-C(152)	1.425(4)
C(12)-H(122)	0.99(2)
C(22)-C(72)	1.380(2)
C(22)-C(32)	1.398(2)
C(32)-C(42)	1.382(2)
C(32)-H(32)	0.93
C(42)-C(52)	1.383(2)
C(42)-H(42)	0.93
C(52)-C(62)	1.381(2)

C(62)-C(72)	1.387(2)
C(62)-H(62)	0.93
C(72)-H(72)	0.93
C(82)-C(132)	1.384(2)
C(82)-C(92)	1.394(2)
C(92)-C(102)	1.374(3)
C(92)-H(92)	0.93
C(102)-C(112)	1.383(3)
C(102)-H(102)	0.93
C(112)-C(122)	1.384(3)
C(122)-C(132)	1.374(3)
C(122)-H(122)	0.93
C(132)-H(132)	0.93
C(142)-H(146)	0.96
C(142)-H(147)	0.96
C(142)-H(148)	0.96
C(152)-H(156)	0.96
C(152)-H(157)	0.96
C(152)-H(158)	0.96

C(11)-N(11)-C(81)	118.48(13)
C(11)-N(11)-H(11)	112(3)
C(81)-N(11)-H(11)	129(3)
C(11)-N(21)-C(21)	120.28(12)
C(11)-N(21)-H(21)	117(2)
C(21)-N(21)-H(21)	123(2)
C(51)-O(11)-C(141)	118.50(14)
C(111)-O(21)-C(151)	117.2(2)
N(11)-C(11)-N(21)	124.63(13)
N(11)-C(11)-H(111)	120.3(10)
N(21)-C(11)-H(111)	115.1(10)
C(71)-C(21)-C(31)	118.30(13)
C(71)-C(21)-N(21)	119.18(12)
C(31)-C(21)-N(21)	122.52(13)
C(41)-C(31)-C(21)	121.20(12)
C(41)-C(31)-H(31)	119.40(8)
C(21)-C(31)-H(31)	119.40(8)
C(31)-C(41)-C(51)	119.58(12)
C(31)-C(41)-H(41)	120.21(8)
C(51)-C(41)-H(41)	120.21(8)
O(11)-C(51)-C(61)	115.44(13)
O(11)-C(51)-C(41)	124.87(13)
C(61)-C(51)-C(41)	119.69(13)
C(71)-C(61)-C(51)	120.36(13)
C(71)-C(61)-H(61)	119.82(8)
C(51)-C(61)-H(61)	119.82(9)
C(61)-C(71)-C(21)	120.81(12)
C(61)-C(71)-H(71)	119.59(8)
C(21)-C(71)-H(71)	119.59(8)
C(131)-C(81)-C(91)	117.70(14)
C(131)-C(81)-N(11)	120.24(13)
C(91)-C(81)-N(11)	122.06(13)
C(101)-C(91)-C(81)	121.45(14)
C(101)-C(91)-H(91)	119.27(9)
C(81)-C(91)-H(91)	119.27(9)
C(111)-C(101)-C(91)	119.94(14)
C(111)-C(101)-H(101)	120.03(9)
C(91)-C(101)-H(101)	120.03(9)
O(21)-C(111)-C(101)	124.6(2)
O(21)-C(111)-C(121)	116.2(2)

C(101)-C(111)-C(121)	119.17(14)
C(131)-C(121)-C(111)	120.4(2)
C(131)-C(121)-H(121)	119.80(10)
C(111)-C(121)-H(121)	119.80(10)
C(121)-C(131)-C(81)	121.23(14)
C(121)-C(131)-H(131)	119.38(10)
C(81)-C(131)-H(131)	119.38(9)
O(11)-C(141)-H(143)	109.47(11)
O(11)-C(141)-H(144)	109.47(11)
H(143)-C(141)-H(144)	109.5
O(11)-C(141)-H(145)	109.47(13)
H(143)-C(141)-H(145)	109.5
H(144)-C(141)-H(145)	109.5
O(21)-C(151)-H(153)	109.47(13)
O(21)-C(151)-H(154)	109.47(14)
H(153)-C(151)-H(154)	109.5
O(21)-C(151)-H(155)	109.5(2)
H(153)-C(151)-H(155)	109.5
H(154)-C(151)-H(155)	109.5
C(12)-N(12)-C(82)	123.28(13)
C(12)-N(12)-H(12)	112(3)
C(82)-N(12)-H(12)	125(3)
C(12)-N(22)-C(22)	123.51(13)
C(12)-N(22)-H(22)	116(3)
C(22)-N(22)-H(22)	120(3)
C(52)-O(12)-C(142)	117.9(2)
C(112)-O(22)-C(152)	117.5(2)
N(12)-C(12)-N(22)	122.05(14)
N(12)-C(12)-H(122)	119.3(11)
N(22)-C(12)-H(122)	118.6(11)
C(72)-C(22)-C(32)	118.3(2)
C(72)-C(22)-N(22)	118.34(14)
C(32)-C(22)-N(22)	123.3(2)
C(42)-C(32)-C(22)	120.2(2)
C(42)-C(32)-H(32)	119.90(9)
C(22)-C(32)-H(32)	119.90(10)
C(32)-C(42)-C(52)	120.74(14)
C(32)-C(42)-H(42)	119.63(9)
C(52)-C(42)-H(42)	119.63(9)
O(12)-C(52)-C(62)	124.3(2)
O(12)-C(52)-C(42)	116.19(14)
C(62)-C(52)-C(42)	119.5(2)
C(52)-C(62)-C(72)	119.6(2)
C(52)-C(62)-H(62)	120.18(10)
C(72)-C(62)-H(62)	120.18(9)
C(22)-C(72)-C(62)	121.56(14)
C(22)-C(72)-H(72)	119.22(9)
C(62)-C(72)-H(72)	119.22(10)
C(132)-C(82)-C(92)	117.4(2)
C(132)-C(82)-N(12)	118.00(13)
C(92)-C(82)-N(12)	124.5(2)
C(102)-C(92)-C(82)	120.9(2)
C(102)-C(92)-H(92)	119.55(10)
C(82)-C(92)-H(92)	119.55(10)
C(92)-C(102)-C(112)	120.8(2)
C(92)-C(102)-H(102)	119.61(10)
C(112)-C(102)-H(102)	119.61(11)
O(22)-C(112)-C(102)	116.8(2)
O(22)-C(112)-C(122)	124.2(2)
C(102)-C(112)-C(122)	119.0(2)

C(132)-C(122)-C(112)	119.8(2)
C(132)-C(122)-H(122)	120.11(10)
C(112)-C(122)-H(122)	120.11(12)
C(122)-C(132)-C(82)	122.2(2)
C(122)-C(132)-H(132)	118.93(10)
C(82)-C(132)-H(132)	118.93(10)
O(12)-C(142)-H(146)	109.47(12)
O(12)-C(142)-H(147)	109.47(13)
H(146)-C(142)-H(147)	109.5
O(12)-C(142)-H(148)	109.47(14)
H(146)-C(142)-H(148)	109.5
H(147)-C(142)-H(148)	109.5
O(22)-C(152)-H(156)	109.47(14)
O(22)-C(152)-H(157)	109.5(2)
H(156)-C(152)-H(157)	109.5
O(22)-C(152)-H(158)	109.5(2)
H(156)-C(152)-H(158)	109.5
H(157)-C(152)-H(158)	109.5

C(81)-N(11)-C(11)-N(21)	178.70(14)
C(21)-N(21)-C(11)-N(11)	179.12(14)
C(11)-N(21)-C(21)-C(71)	143.9(2)
C(11)-N(21)-C(21)-C(31)	-35.9(2)
C(71)-C(21)-C(31)-C(41)	-2.8(2)
N(21)-C(21)-C(31)-C(41)	177.05(13)
C(21)-C(31)-C(41)-C(51)	2.0(2)
C(141)-O(11)-C(51)-C(61)	173.7(2)
C(141)-O(11)-C(51)-C(41)	-5.7(3)
C(31)-C(41)-C(51)-O(11)	179.43(13)
C(31)-C(41)-C(51)-C(61)	0.1(2)
O(11)-C(51)-C(61)-C(71)	179.19(14)
C(41)-C(51)-C(61)-C(71)	-1.4(2)
C(51)-C(61)-C(71)-C(21)	0.6(2)
C(31)-C(21)-C(71)-C(61)	1.4(2)
N(21)-C(21)-C(71)-C(61)	-178.40(13)
C(11)-N(11)-C(81)-C(131)	137.7(2)
C(11)-N(11)-C(81)-C(91)	-41.6(2)
C(131)-C(81)-C(91)-C(101)	-3.3(2)
N(11)-C(81)-C(91)-C(101)	176.01(14)
C(81)-C(91)-C(101)-C(111)	1.2(3)
C(151)-O(21)-C(111)-C(101)	11.1(3)
C(151)-O(21)-C(111)-C(121)	-168.8(2)
C(91)-C(101)-C(111)-O(21)	-178.5(2)
C(91)-C(101)-C(111)-C(121)	1.4(3)
O(21)-C(111)-C(121)-C(131)	178.2(2)
C(101)-C(111)-C(121)-C(131)	-1.6(3)
C(111)-C(121)-C(131)-C(81)	-0.6(3)
C(91)-C(81)-C(131)-C(121)	3.1(2)
N(11)-C(81)-C(131)-C(121)	-176.30(14)
C(82)-N(12)-C(12)-N(22)	174.7(2)
C(22)-N(22)-C(12)-N(12)	179.0(2)
C(12)-N(22)-C(22)-C(72)	152.4(2)
C(12)-N(22)-C(22)-C(32)	-28.9(2)
C(72)-C(22)-C(32)-C(42)	-1.4(2)
N(22)-C(22)-C(32)-C(42)	179.91(14)
C(22)-C(32)-C(42)-C(52)	0.9(2)
C(142)-O(12)-C(52)-C(62)	6.5(3)
C(142)-O(12)-C(52)-C(42)	-174.3(2)
C(32)-C(42)-C(52)-O(12)	-179.40(13)
C(32)-C(42)-C(52)-C(62)	-0.2(2)

O(12)-C(52)-C(62)-C(72)	179.16(14)
C(42)-C(52)-C(62)-C(72)	0.0(2)
C(32)-C(22)-C(72)-C(62)	1.2(2)
N(22)-C(22)-C(72)-C(62)	-179.99(14)
C(52)-C(62)-C(72)-C(22)	-0.5(2)
C(12)-N(12)-C(82)-C(132)	158.7(2)
C(12)-N(12)-C(82)-C(92)	-25.2(3)
C(132)-C(82)-C(92)-C(102)	0.1(3)
N(12)-C(82)-C(92)-C(102)	-175.9(2)
C(82)-C(92)-C(102)-C(112)	0.8(3)
C(152)-O(22)-C(112)-C(102)	-164.7(3)
C(152)-O(22)-C(112)-C(122)	15.3(4)
C(92)-C(102)-C(112)-O(22)	178.8(2)
C(92)-C(102)-C(112)-C(122)	-1.1(3)
O(22)-C(112)-C(122)-C(132)	-179.4(2)
C(102)-C(112)-C(122)-C(132)	0.6(3)
C(112)-C(122)-C(132)-C(82)	0.3(3)
C(92)-C(82)-C(132)-C(122)	-0.7(3)
N(12)-C(82)-C(132)-C(122)	175.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for N,N'-BIS(P-METOXYPHENYL)-FORMAMMIDINE

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(11)	47(1)	67(1)	58(1)	16(1)	24(1)	29(1)
N(21)	50(1)	73(1)	56(1)	20(1)	24(1)	35(1)
O(11)	86(1)	83(1)	76(1)	28(1)	51(1)	49(1)
O(21)	88(1)	102(1)	54(1)	19(1)	24(1)	37(1)
C(11)	42(1)	58(1)	57(1)	13(1)	19(1)	23(1)
C(21)	39(1)	55(1)	49(1)	12(1)	17(1)	20(1)
C(31)	48(1)	51(1)	48(1)	16(1)	19(1)	19(1)
C(41)	52(1)	49(1)	50(1)	12(1)	17(1)	24(1)
C(51)	47(1)	56(1)	50(1)	12(1)	22(1)	21(1)
C(61)	63(1)	59(1)	60(1)	24(1)	32(1)	28(1)
C(71)	56(1)	54(1)	60(1)	21(1)	25(1)	29(1)
C(81)	43(1)	51(1)	53(1)	8(1)	21(1)	20(1)
C(91)	40(1)	64(1)	63(1)	12(1)	22(1)	14(1)
C(101)	45(1)	73(1)	60(1)	7(1)	13(1)	17(1)
C(111)	64(1)	62(1)	48(1)	6(1)	20(1)	25(1)
C(121)	55(1)	77(1)	60(1)	12(1)	31(1)	21(1)
C(131)	39(1)	77(1)	60(1)	9(1)	22(1)	21(1)
C(141)	96(2)	102(2)	77(1)	23(1)	43(1)	67(1)
C(151)	111(2)	137(2)	63(1)	26(1)	10(1)	61(2)
N(12)	55(1)	75(1)	67(1)	20(1)	27(1)	37(1)
N(22)	51(1)	69(1)	70(1)	18(1)	28(1)	32(1)
O(12)	66(1)	71(1)	89(1)	12(1)	46(1)	26(1)
O(22)	189(2)	135(2)	66(1)	32(1)	40(1)	103(2)
C(12)	48(1)	61(1)	73(1)	19(1)	26(1)	28(1)
C(22)	44(1)	49(1)	69(1)	14(1)	25(1)	19(1)
C(32)	42(1)	56(1)	68(1)	8(1)	19(1)	15(1)
C(42)	38(1)	57(1)	82(1)	12(1)	26(1)	16(1)
C(52)	51(1)	46(1)	78(1)	14(1)	36(1)	16(1)
C(62)	53(1)	63(1)	65(1)	11(1)	23(1)	17(1)
C(72)	42(1)	69(1)	71(1)	15(1)	21(1)	23(1)
C(82)	41(1)	57(1)	66(1)	11(1)	17(1)	21(1)
C(92)	58(1)	64(1)	71(1)	12(1)	21(1)	33(1)
C(102)	73(1)	72(1)	72(1)	18(1)	16(1)	41(1)
C(112)	80(1)	76(1)	59(1)	10(1)	15(1)	35(1)
C(122)	89(1)	67(1)	67(1)	7(1)	25(1)	40(1)
C(132)	67(1)	62(1)	71(1)	15(1)	25(1)	35(1)
C(142)	101(2)	111(2)	89(2)	4(1)	50(1)	44(2)
C(152)	237(5)	128(3)	80(2)	33(2)	76(2)	97(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for N,N'-BIS(P-METOXYPHENYL)-FORMAMMIDINE

	x	y	z	U(eq)
H(11)	4811(54)	7544(47)	3822(31)	47(15)
H(21)	4469(37)	7681(31)	5230(21)	50(11)
H(111)	2685(20)	8549(18)	3860(12)	53(4)
H(31)	2749(2)	10104(1)	4983(1)	54(4)
H(41)	1284(2)	10600(1)	5811(1)	54(4)
H(61)	1555(2)	7390(2)	7189(1)	77(6)
H(71)	2937(2)	6851(2)	6321(1)	63(5)
H(91)	1544(2)	7273(2)	2331(1)	60(5)
H(101)	853(2)	7749(2)	811(1)	88(7)
H(121)	5172(2)	9311(2)	1006(1)	74(6)
H(131)	5849(2)	8850(2)	2521(1)	94(7)
H(143)	-567(3)	10451(3)	7495(2)	113(9)
H(144)	-588(3)	10420(3)	6443(2)	90(7)
H(145)	882(3)	11252(3)	7265(2)	113(9)
H(153)	1096(3)	9138(4)	-1225(2)	129(10)
H(154)	886(3)	9496(4)	-254(2)	129(11)
H(155)	498(3)	7943(4)	-680(2)	160(15)
H(12)	5735(53)	7461(47)	5626(31)	70(16)
H(22)	5922(48)	7004(42)	4259(27)	92(15)
H(122)	7861(22)	6337(20)	5723(13)	69(5)
H(32)	9498(2)	6713(2)	4901(1)	63(5)
H(42)	10548(2)	5935(2)	3888(1)	84(6)
H(62)	6737(2)	5088(2)	1751(1)	77(6)
H(72)	5680(2)	5857(2)	2766(1)	71(5)
H(92)	7435(2)	5427(2)	6972(1)	81(6)
H(102)	7679(2)	5237(2)	8524(1)	88(7)
H(122)	6191(2)	8419(2)	8750(1)	76(6)
H(132)	5985(2)	8625(2)	7206(1)	76(6)
H(146)	9366(3)	4323(3)	903(2)	112(8)
H(147)	8534(3)	5394(3)	939(2)	112(9)
H(148)	7823(3)	3860(3)	1084(2)	107(9)
H(156)	6556(6)	7002(4)	10833(2)	160(13)
H(157)	5312(6)	6891(4)	9878(2)	259(32)
H(158)	6750(6)	8215(4)	10234(2)	170(15)

Table 1. Crystal data and structure refinement for N,N'-bis(p-methylphenyl)-formamidine

Empirical formula	C15 H16 N2
Formula weight	224.30
Temperature	293(2) K
Wavelength	1.54178 A
Crystal system	TRICLINIC
Space group	P-1
Unit cell dimensions	a = 6.0990(10) A alpha = 93.17(3) deg. b = 10.519(2) A beta = 96.34(3) deg. c = 10.122(2) A gamma = 80.99(3) deg.
Volume	637.0(2) A^3
Z	2
Density (calculated)	1.169 Mg/m^3
Absorption coefficient	0.535 mm^-1
F(000)	240
Crystal size	0.2 x 0.2 x 0.2 mm
Theta range for data collection	4.26 to 80.20 deg.
Index ranges	-7<=h<=7, -12<=k<=12, 0<=l<=11
Reflections collected	2733
Independent reflections	2542 [R(int) = 0.5168]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2536 / 0 / 176
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0683, wR2 = 0.1725
R indices (all data)	R1 = 0.0874, wR2 = 0.1873
Largest diff. peak and hole	0.380 and -0.441 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for
N,N'-bis(p-methylphenyl)-formamidine
U(eq) is defined
as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	3175(2)	-37(1)	6368(1)	43(1)
C(1)	4612(2)	-1015(1)	6716(1)	43(1)
N(2)	6182(2)	-1579(1)	5946(1)	47(1)
C(2)	1782(2)	533(1)	7345(1)	40(1)
C(3)	2634(2)	791(2)	8653(1)	47(1)
C(4)	1240(3)	1417(2)	9554(1)	51(1)
C(5)	-1004(3)	1826(2)	9191(2)	48(1)
C(6)	-1850(2)	1553(2)	7888(2)	47(1)
C(7)	-481(2)	910(2)	6981(1)	43(1)
C(8)	7772(2)	-2662(1)	6311(1)	44(1)
C(9)	9791(3)	-2845(2)	5776(2)	52(1)
C(10)	11384(3)	-3900(2)	6096(2)	58(1)
C(11)	11042(3)	-4786(2)	6969(2)	57(1)
C(12)	9019(3)	-4598(2)	7494(2)	62(1)
C(13)	7378(3)	-3560(2)	7171(2)	56(1)
C(14)	-2485(3)	2560(2)	10169(2)	66(1)
C(15)	12819(4)	-5920(2)	7326(3)	83(1)

Table 4. Bond lengths [A] and angles [deg] for N,N'-bis(p-methylphenyl)-formamidine

N(1)-C(1)	1.280(2)
N(1)-C(2)	1.421(2)
C(1)-N(2)	1.346(2)
C(1)-H(1)	0.99(2)
N(2)-C(8)	1.413(2)
C(2)-C(7)	1.389(2)
C(2)-C(3)	1.396(2)
C(3)-C(4)	1.385(2)
C(3)-H(3)	0.93
C(4)-C(5)	1.384(2)
C(4)-H(4)	0.93
C(5)-C(6)	1.394(2)
C(5)-C(14)	1.512(2)
C(6)-C(7)	1.386(2)
C(6)-H(6)	0.93
C(7)-H(7)	0.93
C(8)-C(9)	1.380(2)
C(8)-C(13)	1.384(2)
C(9)-C(10)	1.383(2)
C(9)-H(9)	0.93
C(10)-C(11)	1.373(3)
C(10)-H(10)	0.93
C(11)-C(12)	1.379(3)
C(11)-C(15)	1.512(2)
C(12)-C(13)	1.388(2)
C(12)-H(12)	0.93
C(13)-H(13)	0.93
C(14)-H(141)	0.96
C(14)-H(142)	0.96
C(14)-H(143)	0.96
C(15)-H(151)	0.96
C(15)-H(152)	0.96
C(15)-H(153)	0.96

C(1)-N(1)-C(2)	116.53(12)
N(1)-C(1)-N(2)	123.25(13)
N(1)-C(1)-H(1)	120.9(10)
N(2)-C(1)-H(1)	115.8(10)
C(1)-N(2)-C(8)	124.02(13)
C(1)-N(2)-H(2)	117.9(12)
C(8)-N(2)-H(2)	116.6(12)
C(7)-C(2)-C(3)	118.45(13)
C(7)-C(2)-N(1)	119.47(12)
C(3)-C(2)-N(1)	121.99(13)
C(4)-C(3)-C(2)	120.19(14)
C(4)-C(3)-H(3)	119.91(9)
C(2)-C(3)-H(3)	119.91(9)
C(3)-C(4)-C(5)	121.73(14)
C(3)-C(4)-H(4)	119.13(9)
C(5)-C(4)-H(4)	119.13(9)
C(4)-C(5)-C(6)	117.80(14)
C(4)-C(5)-C(14)	121.2(2)
C(6)-C(5)-C(14)	121.0(2)
C(7)-C(6)-C(5)	121.04(14)
C(7)-C(6)-H(6)	119.48(8)

C(5)-C(6)-H(6)	119.48(9)
C(6)-C(7)-C(2)	120.76(13)
C(6)-C(7)-H(7)	119.62(8)
C(2)-C(7)-H(7)	119.62(8)
C(9)-C(8)-C(13)	118.49(14)
C(9)-C(8)-N(2)	118.91(14)
C(13)-C(8)-N(2)	122.59(14)
C(8)-C(9)-C(10)	120.8(2)
C(8)-C(9)-H(9)	119.62(9)
C(10)-C(9)-H(9)	119.62(11)
C(11)-C(10)-C(9)	121.6(2)
C(11)-C(10)-H(10)	119.20(11)
C(9)-C(10)-H(10)	119.20(11)
C(12)-C(11)-C(10)	117.3(2)
C(12)-C(11)-C(15)	121.9(2)
C(10)-C(11)-C(15)	120.9(2)
C(11)-C(12)-C(13)	122.2(2)
C(11)-C(12)-H(12)	118.89(10)
C(13)-C(12)-H(12)	118.89(11)
C(8)-C(13)-C(12)	119.7(2)
C(8)-C(13)-H(13)	120.17(10)
C(12)-C(13)-H(13)	120.17(11)
C(5)-C(14)-H(141)	109.47(10)
C(5)-C(14)-H(142)	109.47(10)
H(141)-C(14)-H(142)	109.5
C(5)-C(14)-H(143)	109.47(10)
H(141)-C(14)-H(143)	109.5
H(142)-C(14)-H(143)	109.5
C(11)-C(15)-H(151)	109.47(14)
C(11)-C(15)-H(152)	109.47(12)
H(151)-C(15)-H(152)	109.5
C(11)-C(15)-H(153)	109.47(12)
H(151)-C(15)-H(153)	109.5
H(152)-C(15)-H(153)	109.5

Symmetry transformations used to generate equivalent atoms:

for deposition

Table. Anisotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-methylphenyl)-formamidine
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)	44(1)	49(1)	35(1)	4(1)	5(1)	0(1)
C(1)	47(1)	45(1)	37(1)	5(1)	5(1)	-2(1)
N(2)	52(1)	47(1)	41(1)	9(1)	9(1)	5(1)
C(2)	43(1)	42(1)	34(1)	5(1)	5(1)	-4(1)
C(3)	44(1)	58(1)	37(1)	5(1)	0(1)	-3(1)
C(4)	55(1)	62(1)	34(1)	-1(1)	3(1)	-7(1)
C(5)	52(1)	50(1)	42(1)	0(1)	13(1)	-9(1)
C(6)	41(1)	53(1)	46(1)	5(1)	5(1)	-4(1)
C(7)	44(1)	50(1)	35(1)	3(1)	2(1)	-7(1)
C(8)	48(1)	40(1)	41(1)	2(1)	1(1)	-2(1)
C(9)	54(1)	51(1)	51(1)	7(1)	10(1)	1(1)
C(10)	51(1)	57(1)	61(1)	0(1)	5(1)	4(1)
C(11)	60(1)	43(1)	62(1)	0(1)	-11(1)	0(1)
C(12)	68(1)	47(1)	69(1)	17(1)	-1(1)	-6(1)
C(13)	55(1)	52(1)	62(1)	12(1)	7(1)	-6(1)
C(14)	65(1)	77(1)	55(1)	-11(1)	22(1)	-6(1)
C(15)	80(1)	54(1)	102(2)	11(1)	-17(1)	12(1)

for deposition

Table. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-methylphenyl)-formamidine

	x	y	z	U(eq)
H(1)	4643(28)	-1391(17)	7591(17)	49(4)
H(2)	6439(31)	-1146(20)	5250(20)	58(5)
H(3)	4142(2)	541(2)	8920(1)	58(5)
H(4)	1828(3)	1567(2)	10426(1)	78(6)
H(6)	-3358(2)	1805(2)	7623(2)	55(5)
H(7)	-1083(2)	730(2)	6119(1)	59(5)
H(9)	10082(3)	-2252(2)	5195(2)	69(6)
H(10)	12719(3)	-4012(2)	5710(2)	78(7)
H(12)	8744(3)	-5188(2)	8084(2)	91(7)
H(13)	6020(3)	-3468(2)	7530(2)	63(5)
H(141)	-3978(3)	2760(2)	9745(2)	167(15)
H(142)	-1929(3)	3344(2)	10463(2)	147(13)
H(143)	-2488(3)	2042(2)	10920(2)	198(18)
H(151)	14098(4)	-5883(2)	6862(3)	258(27)
H(152)	12243(4)	-6707(2)	7074(3)	196(19)
H(153)	13247(4)	-5891(2)	8268(3)	163(15)

Table 1. Crystal data and structure refinement for N,N'-bis(p-fluorophenyl)-formamidine

Empirical formula	C13 H10 F2 N2
Formula weight	232.23
Temperature	293(2) K
Wavelength	1.54178 A
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 10.882(2) A alpha = 69.51(3) deg. b = 10.930(2) A beta = 65.70(3) deg. c = 11.326(2) A gamma = 72.12(3) deg.
Volume	1128.9(4) A^3
Z	4
Density (calculated)	1.366 Mg/m^3
Absorption coefficient	0.892 mm^-1
F(000)	480
Crystal size	0.25 x 0.25 x 0.25 mm
Theta range for data collection	2.40 to 75.10 deg.
Index ranges	0<=h<=12, -11<=k<=11, -11<=l<=11
Reflections collected	3748
Independent reflections	3530 [R(int) = 0.0364]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3506 / 0 / 339
Goodness-of-fit on F^2	0.928
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1156
R indices (all data)	R1 = 0.0655, wR2 = 0.1383
Largest diff. peak and hole	0.164 and -0.207 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-fluorophenyl)-formamidine
U(eq) is defined
as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(11)	1521(2)	8001(2)	9452(2)	47(1)
N(21)	-95(2)	7103(2)	9388(2)	47(1)
F(11)	-4559(1)	4624(2)	11468(2)	80(1)
F(21)	3508(2)	9771(2)	12218(2)	93(1)
C(11)	456(2)	7462(2)	10053(2)	44(1)
C(21)	-1235(2)	6464(2)	9964(2)	42(1)
C(31)	-1774(2)	5886(2)	11325(2)	56(1)
C(41)	-2901(2)	5276(2)	11830(2)	61(1)
C(51)	-3448(2)	5236(2)	10969(2)	55(1)
C(61)	-2925(2)	5750(3)	9626(2)	66(1)
C(71)	-1810(2)	6372(2)	9124(2)	61(1)
C(81)	1982(2)	8422(2)	10225(2)	43(1)
C(91)	1108(2)	9140(2)	11153(2)	50(1)
C(101)	1614(3)	9593(2)	11826(2)	59(1)
C(111)	3000(3)	9318(2)	11561(2)	60(1)
C(121)	3898(3)	8608(3)	10664(2)	67(1)
C(131)	3388(2)	8162(2)	9992(2)	58(1)
N(12)	1270(2)	7885(2)	6303(2)	48(1)
N(22)	2348(2)	9272(2)	6520(2)	47(1)
F(12)	4799(2)	13634(1)	4765(2)	76(1)
F(22)	809(2)	5632(1)	2863(1)	74(1)
C(12)	2083(2)	8715(2)	5780(2)	44(1)
C(22)	3005(2)	10369(2)	6028(2)	41(1)
C(32)	3490(2)	11012(2)	4670(2)	48(1)
C(42)	4098(2)	12110(2)	4247(2)	53(1)
C(52)	4216(2)	12540(2)	5182(2)	53(1)
C(62)	3778(2)	11920(2)	6516(2)	57(1)
C(72)	3159(2)	10830(2)	6940(2)	51(1)
C(82)	1186(2)	7303(2)	5401(2)	42(1)
C(92)	2322(2)	6564(2)	4640(2)	53(1)
C(102)	2206(2)	6004(2)	3782(2)	57(1)
C(112)	935(2)	6187(2)	3705(2)	50(1)
C(122)	-210(2)	6898(2)	4438(2)	53(1)
C(132)	-81(2)	7452(2)	5291(2)	48(1)

Table 4. Bond lengths [A] and angles [deg] for N,N'-bis(p-fluorophenyl)-formamidine

N(11)-C(11)	1.283(3)
N(11)-C(81)	1.418(2)
N(21)-C(11)	1.342(2)
N(21)-C(21)	1.414(2)
N(21)-H(111)	0.87(2)
F(11)-C(51)	1.377(2)
F(21)-C(111)	1.367(2)
C(11)-H(11)	0.95(2)
C(21)-C(71)	1.380(3)
C(21)-C(31)	1.386(3)
C(31)-C(41)	1.391(3)
C(31)-H(31)	0.93
C(41)-C(51)	1.354(3)
C(41)-H(41)	0.93
C(51)-C(61)	1.356(3)
C(61)-C(71)	1.388(3)
C(61)-H(61)	0.93
C(71)-H(71)	0.93
C(81)-C(91)	1.387(3)
C(81)-C(131)	1.395(3)
C(91)-C(101)	1.380(3)
C(91)-H(91)	0.93
C(101)-C(111)	1.366(3)
C(101)-H(101)	0.93
C(111)-C(121)	1.363(4)
C(121)-C(131)	1.378(3)
C(121)-H(121)	0.93
C(131)-H(131)	0.93
N(12)-C(12)	1.281(3)
N(12)-C(82)	1.423(2)
N(22)-C(12)	1.349(2)
N(22)-C(22)	1.410(2)
N(22)-H(222)	0.84(2)
F(12)-C(52)	1.371(2)
F(22)-C(112)	1.363(2)
C(12)-H(12)	0.96(2)
C(22)-C(32)	1.393(3)
C(22)-C(72)	1.382(3)
C(32)-C(42)	1.390(3)
C(32)-H(32)	0.93
C(42)-C(52)	1.363(3)
C(42)-H(42)	0.93
C(52)-C(62)	1.363(3)
C(62)-C(72)	1.388(3)
C(62)-H(62)	0.93
C(72)-H(72)	0.93
C(82)-C(92)	1.386(3)
C(82)-C(132)	1.390(3)
C(92)-C(102)	1.379(3)
C(92)-H(92)	0.93
C(102)-C(112)	1.370(3)
C(102)-H(102)	0.93
C(112)-C(122)	1.361(3)
C(122)-C(132)	1.376(3)
C(122)-H(122)	0.93

C(132)-H(132)	0.93
C(11)-N(11)-C(81)	118.2(2)
C(11)-N(21)-C(21)	126.3(2)
C(11)-N(21)-H(111)	117.5(14)
C(21)-N(21)-H(111)	116.2(14)
N(11)-C(11)-N(21)	122.2(2)
N(11)-C(11)-H(11)	121.9(12)
N(21)-C(11)-H(11)	116.0(12)
C(71)-C(21)-C(31)	118.4(2)
C(71)-C(21)-N(21)	118.4(2)
C(31)-C(21)-N(21)	123.2(2)
C(21)-C(31)-C(41)	120.4(2)
C(21)-C(31)-H(31)	119.78(12)
C(41)-C(31)-H(31)	119.78(13)
C(51)-C(41)-C(31)	119.0(2)
C(51)-C(41)-H(41)	120.52(12)
C(31)-C(41)-H(41)	120.52(13)
C(61)-C(51)-C(41)	122.5(2)
C(61)-C(51)-F(11)	118.6(2)
C(41)-C(51)-F(11)	118.9(2)
C(51)-C(61)-C(71)	118.5(2)
C(51)-C(61)-H(61)	120.73(13)
C(71)-C(61)-H(61)	120.73(13)
C(21)-C(71)-C(61)	121.2(2)
C(21)-C(71)-H(71)	119.42(12)
C(61)-C(71)-H(71)	119.42(13)
C(91)-C(81)-C(131)	118.2(2)
C(91)-C(81)-N(11)	123.2(2)
C(131)-C(81)-N(11)	118.5(2)
C(81)-C(91)-C(101)	121.0(2)
C(81)-C(91)-H(91)	119.48(12)
C(101)-C(91)-H(91)	119.48(14)
C(111)-C(101)-C(91)	118.6(2)
C(111)-C(101)-H(101)	120.70(13)
C(91)-C(101)-H(101)	120.70(13)
C(121)-C(111)-C(101)	122.5(2)
C(121)-C(111)-F(21)	118.6(2)
C(101)-C(111)-F(21)	118.9(2)
C(111)-C(121)-C(131)	118.6(2)
C(111)-C(121)-H(121)	120.68(14)
C(131)-C(121)-H(121)	120.68(14)
C(121)-C(131)-C(81)	121.0(2)
C(121)-C(131)-H(131)	119.52(14)
C(81)-C(131)-H(131)	119.52(12)
C(12)-N(12)-C(82)	115.9(2)
C(12)-N(22)-C(22)	126.1(2)
C(12)-N(22)-H(222)	119(2)
C(22)-N(22)-H(222)	115(2)
N(12)-C(12)-N(22)	122.6(2)
N(12)-C(12)-H(12)	120.9(12)
N(22)-C(12)-H(12)	116.4(12)
C(32)-C(22)-C(72)	118.8(2)
C(32)-C(22)-N(22)	123.0(2)
C(72)-C(22)-N(22)	118.2(2)
C(22)-C(32)-C(42)	120.4(2)
C(22)-C(32)-H(32)	119.78(11)
C(42)-C(32)-H(32)	119.78(13)
C(52)-C(42)-C(32)	118.8(2)
C(52)-C(42)-H(42)	120.59(12)

C(32)-C(42)-H(42)	120.59(13)
C(62)-C(52)-C(42)	122.3(2)
C(62)-C(52)-F(12)	118.9(2)
C(42)-C(52)-F(12)	118.8(2)
C(52)-C(62)-C(72)	118.9(2)
C(52)-C(62)-H(62)	120.57(12)
C(72)-C(62)-H(62)	120.57(13)
C(22)-C(72)-C(62)	120.8(2)
C(22)-C(72)-H(72)	119.61(11)
C(62)-C(72)-H(72)	119.61(13)
C(92)-C(82)-C(132)	118.3(2)
C(92)-C(82)-N(12)	122.4(2)
C(132)-C(82)-N(12)	119.3(2)
C(82)-C(92)-C(102)	121.0(2)
C(82)-C(92)-H(92)	119.49(12)
C(102)-C(92)-H(92)	119.49(13)
C(112)-C(102)-C(92)	118.4(2)
C(112)-C(102)-H(102)	120.80(13)
C(92)-C(102)-H(102)	120.80(13)
C(122)-C(112)-F(22)	118.6(2)
C(122)-C(112)-C(102)	122.6(2)
F(22)-C(112)-C(102)	118.8(2)
C(112)-C(122)-C(132)	118.5(2)
C(112)-C(122)-H(122)	120.76(12)
C(132)-C(122)-H(122)	120.76(12)
C(122)-C(132)-C(82)	121.2(2)
C(122)-C(132)-H(132)	119.41(12)
C(82)-C(132)-H(132)	119.41(12)

for deposition

Table . Anisotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-fluorophenyl)-formamidine

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(11)	51(1)	54(1)	41(1)	-11(1)	-12(1)	-23(1)
N(21)	52(1)	55(1)	36(1)	-11(1)	-10(1)	-24(1)
F(11)	63(1)	101(1)	83(1)	-26(1)	-5(1)	-49(1)
F(21)	115(1)	126(1)	76(1)	-33(1)	-40(1)	-57(1)
C(11)	52(1)	44(1)	37(1)	-8(1)	-14(1)	-14(1)
C(21)	41(1)	41(1)	43(1)	-13(1)	-8(1)	-13(1)
C(31)	63(1)	67(1)	44(1)	-12(1)	-13(1)	-30(1)
C(41)	64(1)	72(2)	46(1)	-11(1)	-5(1)	-34(1)
C(51)	45(1)	59(1)	61(1)	-20(1)	-3(1)	-26(1)
C(61)	64(1)	87(2)	60(1)	-19(1)	-20(1)	-35(1)
C(71)	67(1)	82(2)	44(1)	-11(1)	-15(1)	-38(1)
C(81)	51(1)	46(1)	35(1)	-5(1)	-15(1)	-19(1)
C(91)	54(1)	51(1)	48(1)	-12(1)	-15(1)	-16(1)
C(101)	77(2)	56(1)	49(1)	-19(1)	-19(1)	-17(1)
C(111)	80(2)	70(1)	47(1)	-11(1)	-27(1)	-35(1)
C(121)	58(1)	92(2)	62(1)	-19(1)	-21(1)	-28(1)
C(131)	53(1)	75(2)	54(1)	-24(1)	-14(1)	-19(1)
N(12)	51(1)	57(1)	42(1)	-14(1)	-10(1)	-25(1)
N(22)	54(1)	57(1)	37(1)	-13(1)	-10(1)	-26(1)
F(12)	74(1)	63(1)	102(1)	-8(1)	-34(1)	-39(1)
F(22)	115(1)	70(1)	64(1)	-22(1)	-44(1)	-29(1)
C(12)	46(1)	50(1)	39(1)	-14(1)	-11(1)	-16(1)
C(22)	34(1)	45(1)	45(1)	-14(1)	-10(1)	-13(1)
C(32)	44(1)	56(1)	48(1)	-17(1)	-11(1)	-16(1)
C(42)	46(1)	56(1)	55(1)	-8(1)	-11(1)	-20(1)
C(52)	40(1)	48(1)	72(2)	-11(1)	-17(1)	-19(1)
C(62)	59(1)	58(1)	69(2)	-23(1)	-27(1)	-16(1)
C(72)	55(1)	57(1)	47(1)	-15(1)	-15(1)	-21(1)
C(82)	48(1)	45(1)	37(1)	-7(1)	-14(1)	-18(1)
C(92)	47(1)	66(1)	53(1)	-21(1)	-17(1)	-13(1)
C(102)	62(1)	58(1)	54(1)	-23(1)	-19(1)	-7(1)
C(112)	75(1)	45(1)	42(1)	-6(1)	-27(1)	-22(1)
C(122)	56(1)	59(1)	52(1)	-6(1)	-25(1)	-23(1)
C(132)	45(1)	55(1)	46(1)	-13(1)	-14(1)	-15(1)

for deposition

Table. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-fluorophenyl)-formamidine

	x	y	z	U(eq)
H(111)	292(22)	7260(21)	8520(23)	50(6)
H(11)	3(20)	7304(18)	10990(20)	39(5)
H(31)	-1379(2)	5907(2)	11905(2)	56(6)
H(41)	-3273(2)	4900(2)	12745(2)	86(8)
H(61)	-3306(2)	5687(3)	9054(2)	95(9)
H(71)	-1445(2)	6733(2)	8205(2)	78(8)
H(91)	167(2)	9320(2)	11325(2)	63(7)
H(101)	1024(3)	10076(2)	12446(2)	74(7)
H(121)	4836(3)	8429(3)	10508(2)	82(8)
H(131)	3991(2)	7681(2)	9373(2)	79(8)
H(222)	2122(22)	8942(21)	7351(23)	50(6)
H(12)	2524(21)	8988(20)	4822(22)	49(5)
H(32)	3407(2)	10704(2)	4043(2)	67(7)
H(42)	4419(2)	12543(2)	3341(2)	70(7)
H(62)	3891(2)	12221(2)	7131(2)	77(8)
H(72)	2845(2)	10406(2)	7849(2)	53(6)
H(92)	3176(2)	6444(2)	4709(2)	70(7)
H(102)	2971(2)	5514(2)	3267(2)	74(7)
H(122)	-1060(2)	7007(2)	4365(2)	68(7)
H(132)	-856(2)	7935(2)	5803(2)	80(8)

Table 1. Crystal data and structure refinement for N,N'-bis(p-nitrophenyl)-formamidine.

Empirical formula	C13 H10 N4 O4
Formula weight	286.25
Temperature	293(2) K
Wavelength	1.54178 A
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 7.674(2) A alpha = 76.28(3) deg. b = 8.575(2) A beta = 79.46(3) deg. c = 10.489(2) A gamma = 78.13(3) deg.
Volume	649.6(3) A^3
Z	2
Density (calculated)	1.463 Mg/m^3
Absorption coefficient	0.949 mm^-1
F(000)	296
Crystal size	0.25 x 0.25 x 0.30 mm
Theta range for data collection	4.38 to 69.96 deg.
Index ranges	-9<=h<=8, -10<=k<=9, -12<=l<=0
Reflections collected	1618
Independent reflections	1594 [R(int) = 0.1031]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1587 / 0 / 200
Goodness-of-fit on F^2	0.988
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1449
R indices (all data)	R1 = 0.1071, wR2 = 0.1775
Largest diff. peak and hole	0.163 and -0.248 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-nitrophenyl)-formamidine U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	4994(4)	8299(3)	1436(3)	57(1)
C(1)	3770(4)	7891(4)	960(3)	53(1)
N(2)	3039(4)	8842(3)	-110(3)	54(1)
C(2)	1593(4)	8512(4)	-588(3)	48(1)
C(3)	599(5)	7333(4)	109(4)	59(1)
C(4)	-810(5)	7061(4)	-380(4)	60(1)
C(5)	-1280(4)	7959(4)	-1558(4)	60(1)
C(6)	-339(6)	9180(5)	-2278(4)	71(1)
C(7)	1116(5)	9430(4)	-1771(3)	60(1)
C(8)	5726(4)	7126(4)	2489(3)	47(1)
C(9)	6264(5)	5499(4)	2423(4)	56(1)
C(10)	7093(5)	4421(5)	3412(4)	65(1)
C(11)	7379(4)	4979(5)	4463(3)	62(1)
C(12)	6825(5)	6577(5)	4571(3)	64(1)
C(13)	5996(5)	7638(5)	3578(3)	57(1)
N(3)	8317(5)	3837(6)	5505(4)	94(1)
O(1)	8539(4)	4343(5)	6443(3)	119(2)
O(2)	8835(6)	2442(6)	5372(4)	142(2)
N(4)	-2840(5)	7685(5)	-2040(5)	87(1)
O(3)	-3301(5)	8579(4)	-3059(4)	130(2)
O(4)	-3577(4)	6546(5)	-1398(4)	115(1)

Table 4. Bond lengths [A] and angles [deg] for N,N'-bis(p-nitrophenyl)-formamidine

N(1)-C(1)	1.282(4)
N(1)-C(8)	1.419(4)
C(1)-N(2)	1.360(4)
C(1)-H(2)	0.93
N(2)-C(2)	1.401(4)
N(2)-H(22)	0.99(5)
C(2)-C(7)	1.371(4)
C(2)-C(3)	1.379(5)
C(3)-C(4)	1.360(5)
C(3)-H(3)	0.93
C(4)-C(5)	1.359(5)
C(4)-H(4)	0.93
C(5)-C(6)	1.388(6)
C(5)-N(4)	1.461(5)
C(6)-C(7)	1.395(5)
C(6)-H(6)	0.93
C(7)-H(7)	0.93
C(8)-C(13)	1.380(5)
C(8)-C(9)	1.386(5)
C(9)-C(10)	1.371(5)
C(9)-H(9)	0.93
C(10)-C(11)	1.370(5)
C(10)-H(10)	0.93
C(11)-C(12)	1.374(5)
C(11)-N(3)	1.471(5)
C(12)-C(13)	1.368(5)
C(12)-H(12)	0.93
C(13)-H(13)	0.93
N(3)-O(2)	1.213(6)
N(3)-O(1)	1.215(6)
N(4)-O(3)	1.222(5)
N(4)-O(4)	1.226(5)
C(1)-N(1)-C(8)	115.6(3)
N(1)-C(1)-N(2)	122.0(3)
N(1)-C(1)-H(2)	119.0(2)
N(2)-C(1)-H(2)	119.0(2)
C(1)-N(2)-C(2)	123.7(3)
C(1)-N(2)-H(22)	119(2)
C(2)-N(2)-H(22)	117(2)
C(7)-C(2)-C(3)	118.9(3)
C(7)-C(2)-N(2)	118.7(3)
C(3)-C(2)-N(2)	122.4(3)
C(4)-C(3)-C(2)	120.7(3)
C(4)-C(3)-H(3)	119.7(2)
C(2)-C(3)-H(3)	119.7(2)
C(5)-C(4)-C(3)	120.7(4)
C(5)-C(4)-H(4)	119.7(2)
C(3)-C(4)-H(4)	119.7(2)
C(4)-C(5)-C(6)	120.5(3)
C(4)-C(5)-N(4)	119.7(4)
C(6)-C(5)-N(4)	119.7(4)
C(5)-C(6)-C(7)	118.1(3)
C(5)-C(6)-H(6)	121.0(2)
C(7)-C(6)-H(6)	121.0(2)

C(2)-C(7)-C(6)	121.1(3)
C(2)-C(7)-H(7)	119.4(2)
C(6)-C(7)-H(7)	119.4(2)
C(13)-C(8)-C(9)	119.1(3)
C(13)-C(8)-N(1)	118.9(3)
C(9)-C(8)-N(1)	121.9(3)
C(10)-C(9)-C(8)	120.4(4)
C(10)-C(9)-H(9)	119.8(3)
C(8)-C(9)-H(9)	119.8(2)
C(11)-C(10)-C(9)	118.9(4)
C(11)-C(10)-H(10)	120.5(2)
C(9)-C(10)-H(10)	120.5(3)
C(10)-C(11)-C(12)	122.0(3)
C(10)-C(11)-N(3)	119.1(4)
C(12)-C(11)-N(3)	118.9(4)
C(13)-C(12)-C(11)	118.4(4)
C(13)-C(12)-H(12)	120.8(3)
C(11)-C(12)-H(12)	120.8(2)
C(12)-C(13)-C(8)	121.1(4)
C(12)-C(13)-H(13)	119.4(3)
C(8)-C(13)-H(13)	119.4(2)
O(2)-N(3)-O(1)	123.8(4)
O(2)-N(3)-C(11)	117.8(5)
O(1)-N(3)-C(11)	118.4(5)
O(3)-N(4)-O(4)	124.5(4)
O(3)-N(4)-C(5)	118.3(5)
O(4)-N(4)-C(5)	117.2(4)

Symmetry transformations used to generate equivalent atoms:

for deposition

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-nitrophenol)-formamidine

	x	y	z	U(eq)
H(2)	3369(4)	6914(4)	1360(3)	61(10)
H(22)	3560(55)	9811(54)	-596(42)	95(13)
H(3)	894(5)	6718(4)	922(4)	81(12)
H(4)	-1458(5)	6251(4)	96(4)	80(12)
H(6)	-669(6)	9814(5)	-3076(4)	84(12)
H(7)	1775(5)	10233(4)	-2245(3)	91(13)
H(9)	6060(5)	5135(4)	1704(4)	64(11)
H(10)	7456(5)	3329(5)	3369(4)	67(11)
H(12)	7009(5)	6929(5)	5302(3)	92(14)
H(13)	5609(5)	8723(5)	3639(3)	60(10)

for deposition

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for N,N'-bis(p-nitrophenyl)-formamidine
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)	62(2)	56(2)	58(2)	-2(1)	-24(2)	-19(1)
C(1)	58(2)	51(2)	52(2)	-4(2)	-14(2)	-17(2)
N(2)	60(2)	49(2)	56(2)	3(2)	-23(1)	-16(1)
C(2)	47(2)	42(2)	59(2)	-13(2)	-19(2)	-4(2)
C(3)	62(2)	50(2)	70(2)	-7(2)	-23(2)	-12(2)
C(4)	57(2)	56(2)	72(2)	-16(2)	-16(2)	-15(2)
C(5)	51(2)	51(2)	90(3)	-28(2)	-27(2)	-2(2)
C(6)	91(3)	56(2)	66(2)	-12(2)	-40(2)	9(2)
C(7)	77(2)	48(2)	61(2)	-3(2)	-22(2)	-20(2)
C(8)	44(2)	49(2)	47(2)	2(2)	-16(2)	-14(2)
C(9)	59(2)	54(2)	55(2)	1(2)	-16(2)	-16(2)
C(10)	56(2)	53(2)	72(3)	8(2)	-6(2)	-9(2)
C(11)	43(2)	82(3)	45(2)	19(2)	-8(2)	-13(2)
C(12)	54(2)	95(3)	43(2)	0(2)	-13(2)	-22(2)
C(13)	53(2)	60(3)	59(2)	-6(2)	-18(2)	-8(2)
N(3)	52(2)	125(4)	77(3)	41(3)	-15(2)	-17(2)
O(1)	74(2)	197(4)	62(2)	35(2)	-27(2)	-26(2)
O(2)	140(3)	103(3)	147(4)	53(3)	-61(3)	4(3)
N(4)	72(2)	74(3)	135(3)	-55(2)	-49(2)	10(2)
O(3)	145(3)	99(3)	179(4)	-55(2)	-123(3)	29(2)
O(4)	78(2)	123(3)	180(4)	-72(3)	-41(2)	-28(2)

Table 1. Crystal data and structure refinement for N,N'-bis(m-bromophenyl)-formamidine.

Empirical formula	C13 H10 Br2 N2
Formula weight	354.05
Temperature	293(2) K
Wavelength	1.54178 A
Crystal system	orthorombic
Space group	Pbca
Unit cell dimensions	a = 7.4590(10) A alpha = 90 deg. b = 14.509(3) A beta = 90 deg. c = 23.751(5) A gamma = 90 deg.
Volume	2570.4(8) A^3
Z	8
Density (calculated)	1.830 Mg/m^3
Absorption coefficient	7.819 mm^-1
F(000)	1376
Crystal size	0.3 x 0.2 x 0.05 mm
Theta range for data collection	3.72 to 70.18 deg.
Index ranges	0<=h<=9, 0<=k<=16, 0<=l<=25
Reflections collected	2178
Independent reflections	2178 [R(int) = 0.0000]
Max. and min. transmission	1.02 and 0.99
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2165 / 0 / 195
Goodness-of-fit on F^2	1.109
Final R indices [I>2sigma(I)]	R1 = 0.0751, wR2 = 0.2377
R indices (all data)	R1 = 0.0819, wR2 = 0.2669
Extinction coefficient	0.0000(2)
Largest diff. peak and hole	0.807 and -0.740 e.A^-3
Absorption correction:empirical	T(min)= 0.99, T(max) = 1.02

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) N,N'-bis(m-bromophenyl)-formamidine. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	-6434(1)	7952(1)	6248(1)	104(1)
Br(2)	1168(1)	8633(1)	2213(1)	105(1)
N(1)	-42(7)	10116(3)	4201(2)	80(1)
N(2)	-2227(7)	9443(4)	4765(2)	82(1)
C(1)	-1522(8)	9658(5)	4255(3)	81(2)
C(2)	-3882(8)	9017(4)	4847(3)	78(2)
C(3)	-5137(9)	8879(5)	4426(3)	86(2)
C(4)	-6760(10)	8438(5)	4552(4)	91(2)
C(5)	-7201(9)	8181(5)	5079(3)	90(2)
C(6)	-5925(8)	8337(5)	5502(3)	84(2)
C(7)	-4330(9)	8766(4)	5399(3)	78(1)
C(8)	546(8)	10228(5)	3641(3)	82(2)
C(9)	1118(9)	11102(6)	3458(4)	89(2)
C(10)	1723(11)	11205(6)	2922(4)	101(2)
C(11)	1780(11)	10497(6)	2543(4)	97(2)
C(12)	1226(8)	9633(6)	2726(3)	88(2)
C(13)	632(8)	9489(5)	3269(3)	81(2)

Table 4. Bond lengths [A], angles [deg] and torsion angles [deg] for N,N'-bis(m-bromophenyl)-formamidine.

Br(1)-C(6)	1.896(8)
Br(2)-C(12)	1.896(8)
N(1)-C(1)	1.296(8)
N(1)-C(8)	1.410(8)
N(2)-C(1)	1.356(8)
N(2)-C(2)	1.394(8)
N(2)-H(2)	0.81(6)
C(1)-H(1)	0.94(9)
C(2)-C(3)	1.385(10)
C(2)-C(7)	1.401(10)
C(3)-C(4)	1.401(10)
C(3)-H(3)	0.92(10)
C(4)-C(5)	1.348(11)
C(4)-H(4)	1.05(10)
C(5)-C(6)	1.401(10)
C(5)-H(5)	1.14(6)
C(6)-C(7)	1.365(9)
C(7)-H(7)	0.84(8)
C(8)-C(13)	1.392(10)
C(8)-C(9)	1.407(10)
C(9)-C(10)	1.358(13)
C(9)-H(9)	0.88(6)
C(10)-C(11)	1.367(13)
C(10)-H(10)	0.97(8)
C(11)-C(12)	1.390(11)
C(11)-H(11)	0.88(8)
C(12)-C(13)	1.380(9)
C(13)-H(13)	1.00(7)

C(1)-N(1)-C(8)	114.7(5)
C(1)-N(2)-C(2)	124.7(6)
C(1)-N(2)-H(2)	118(4)
C(2)-N(2)-H(2)	117(4)
N(1)-C(1)-N(2)	122.4(6)
N(1)-C(1)-H(1)	126(5)
N(2)-C(1)-H(1)	111(5)
C(3)-C(2)-N(2)	124.2(6)
C(3)-C(2)-C(7)	118.5(6)
N(2)-C(2)-C(7)	117.2(6)
C(2)-C(3)-C(4)	119.7(7)
C(2)-C(3)-H(3)	114(6)
C(4)-C(3)-H(3)	126(6)
C(5)-C(4)-C(3)	122.4(7)
C(5)-C(4)-H(4)	126(6)
C(3)-C(4)-H(4)	112(6)
C(4)-C(5)-C(6)	117.0(6)
C(4)-C(5)-H(5)	130(3)
C(6)-C(5)-H(5)	113(3)
C(7)-C(6)-C(5)	122.5(7)
C(7)-C(6)-Br(1)	118.5(6)
C(5)-C(6)-Br(1)	119.0(5)
C(6)-C(7)-C(2)	119.6(7)
C(6)-C(7)-H(7)	118(5)
C(2)-C(7)-H(7)	122(5)
C(13)-C(8)-C(9)	118.9(6)
C(13)-C(8)-N(1)	121.7(6)

C(9)-C(8)-N(1)	119.4(6)
C(10)-C(9)-C(8)	119.3(8)
C(10)-C(9)-H(9)	128(4)
C(8)-C(9)-H(9)	112(4)
C(9)-C(10)-C(11)	123.1(8)
C(9)-C(10)-H(10)	116(4)
C(11)-C(10)-H(10)	120(4)
C(10)-C(11)-C(12)	117.5(7)
C(10)-C(11)-H(11)	120(6)
C(12)-C(11)-H(11)	122(6)
C(13)-C(12)-C(11)	121.7(8)
C(13)-C(12)-Br(2)	118.5(6)
C(11)-C(12)-Br(2)	119.7(6)
C(12)-C(13)-C(8)	119.4(7)
C(12)-C(13)-H(13)	124(4)
C(8)-C(13)-H(13)	116(4)

C(8)-N(1)-C(1)-N(2)	176.4(6)
C(2)-N(2)-C(1)-N(1)	174.6(6)
C(1)-N(2)-C(2)-C(3)	-9.9(10)
C(1)-N(2)-C(2)-C(7)	174.1(6)
N(2)-C(2)-C(3)-C(4)	179.7(6)
C(7)-C(2)-C(3)-C(4)	-4.3(10)
C(2)-C(3)-C(4)-C(5)	3.6(11)
C(3)-C(4)-C(5)-C(6)	-2.7(11)
C(4)-C(5)-C(6)-C(7)	2.9(10)
C(4)-C(5)-C(6)-Br(1)	-177.9(5)
C(5)-C(6)-C(7)-C(2)	-3.9(10)
Br(1)-C(6)-C(7)-C(2)	176.9(5)
C(3)-C(2)-C(7)-C(6)	4.5(9)
N(2)-C(2)-C(7)-C(6)	-179.2(6)
C(1)-N(1)-C(8)-C(13)	-48.5(8)
C(1)-N(1)-C(8)-C(9)	133.8(6)
C(13)-C(8)-C(9)-C(10)	0.6(10)
N(1)-C(8)-C(9)-C(10)	178.5(7)
C(8)-C(9)-C(10)-C(11)	1.1(12)
C(9)-C(10)-C(11)-C(12)	-1.5(12)
C(10)-C(11)-C(12)-C(13)	0.2(11)
C(10)-C(11)-C(12)-Br(2)	177.2(6)
C(11)-C(12)-C(13)-C(8)	1.5(10)
Br(2)-C(12)-C(13)-C(8)	-175.6(5)
C(9)-C(8)-C(13)-C(12)	-1.9(10)
N(1)-C(8)-C(13)-C(12)	-179.7(6)

Symmetry transformations used to generate equivalent atoms:

for deposition

Table. Anisotropic displacement parameters (Å^2 x 10^3) for N,N'-bis(m-bromophenyl)-formamidine.
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
Br(1)	105(1)	101(1)	106(1)	12(1)	19(1)	-5(1)
Br(2)	102(1)	114(1)	98(1)	-9(1)	9(1)	5(1)
N(1)	83(3)	70(3)	88(3)	4(2)	1(2)	-2(2)
N(2)	84(3)	80(3)	81(3)	-3(2)	0(2)	-11(2)
C(1)	78(3)	81(4)	83(4)	1(3)	2(3)	2(3)
C(2)	78(3)	60(3)	95(4)	0(3)	3(3)	0(2)
C(3)	84(4)	80(4)	94(4)	4(3)	-1(3)	0(3)
C(4)	88(4)	83(4)	102(5)	-5(4)	-7(3)	-4(3)
C(5)	83(4)	74(4)	112(5)	1(3)	8(3)	-4(3)
C(6)	84(3)	69(3)	101(4)	-10(3)	12(3)	-3(3)
C(7)	80(3)	72(3)	83(4)	0(3)	0(3)	-2(3)
C(8)	76(3)	85(4)	85(3)	5(3)	-3(3)	-3(3)
C(9)	84(4)	81(4)	101(5)	7(4)	0(3)	-5(3)
C(10)	98(5)	88(5)	119(6)	26(5)	8(4)	5(4)
C(11)	95(4)	99(5)	98(5)	20(4)	12(4)	2(4)
C(12)	81(3)	95(5)	88(4)	8(3)	3(3)	5(3)
C(13)	75(3)	87(4)	82(3)	18(3)	4(2)	-3(3)

for deposition

Table. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for N,N'-bis(m-bromophenyl)-formamidine

	x	y	z	U(eq)
H(2)	-1668(73)	9589(40)	5044(26)	58(14)
H(1)	-2340(118)	9532(51)	3966(36)	107(23)
H(3)	-4762(137)	9055(62)	4074(41)	123(29)
H(4)	-7563(155)	8355(68)	4194(39)	141(32)
H(5)	-8528(75)	7910(43)	5252(27)	70(17)
H(7)	-3596(89)	8803(53)	5665(35)	85(21)
H(9)	1171(71)	11507(46)	3736(26)	59(15)
H(10)	1940(105)	11833(54)	2800(30)	91(20)
H(11)	2325(121)	10573(57)	2219(35)	111(27)
H(13)	323(96)	8872(49)	3429(30)	85(17)