Table 1. Crystal data and structure refinement for guanidinocarbonyl-1H-pyrrole acetate

Identification code	Guanidiniocarbonyl-1H-pyrrole acetate
Empirical formula	C8 H12 N4 O3 x H2 O
Formula weight	230.23
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 8.360(1) A alpha = 103.18(1) d. b = 8.462(1) A beta = 105.09(1) d. c = 8.558(1) A gamma = 93.46(1) d.
Volume	564.51(12) A^3
Z	2
Density (calculated)	1.354 g/cm^3
Absorption coefficient	0.110 mm^-1
F(000)	244
Crystal size	0.25 x 0.20 x 0.15 mm
Theta range for data collection	2.55 to 27.50 deg.
Index ranges	-10<=h<=10, -10<=k<=10, -11<=l<=11
Reflections collected	4483
Independent reflections	2504 [R(int) = 0.0210]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2504 / 0 / 201
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0960,
Reflection observed [I>2sigma(I)]	2069
R indices (all data)	R1 = 0.0464, wR2 = 0.1027
Largest diff. peak and hole	0.177 and -0.173 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for guanidiniocarbonyl-1H-pyrrole acetate. U(eq) is defined as one third of the trace

of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	-3170(1)	4977(1)	-5376(1)	44(1)
C(2)	-1742(1)	5276(1)	-4073(1)	38(1)
C(3)	-1086(2)	6883(2)	-3790(2)	45(1)
C(4)	-2154(2)	7561(2)	-4949(2)	51(1)
C(5)	-3416(2)	6356(2)	-5904(2)	50(1)
C(6)	-1220(1)	3990(2)	-3258(2)	39(1)
N(7)	297(1)	4421(1)	-2023(1)	38(1)
C(8)	1106(1)	3450(1)	-1076(2)	37(1)
N(9)	2579(1)	4088(2)	-27(1)	46(1)
N(10)	457(2)	1969(1)	-1180(2)	50(1)
O(11)	-2040(1)	2646(1)	-3604(1)	57(1)
O(12)	4542(1)	2439(1)	2014(1)	45(1)
O(13)	2598(1)	283(1)	860(1)	49(1)
C(14)	4000(1)	962(1)	1813(2)	38(1)
C(15)	5128(2)	-44(2)	2746(2)	59(1)
O(16)	2710(1)	-2820(1)	-813(1)	54(1)

Table 3. Bond lengths [A] and angles [deg] for guanidinio-carbonyl-1H-pyrrole acetate.

N(1)-C(5)	1.3517(18)
N(1)-C(2)	1.3689(15)
C(2)-C(3)	1.3775(17)
C(2)-C(6)	1.4519(17)
C(3)-C(4)	1.4041(19)
C(4)-C(5)	1.364(2)
C(6)-O(11)	1.2237(15)
C(6)-N(7)	1.3892(15)
N(7)-C(8)	1.3690(16)
C(8)-N(10)	1.3096(16)
C(8)-N(9)	1.3177(16)
O(12)-C(14)	1.2615(14)
O(13)-C(14)	1.2551(14)
C(14)-C(15)	1.5056(18)
C(5)-N(1)-C(2)	109.08(11)
N(1)-C(2)-C(3)	107.55(11)
N(1)-C(2)-C(6)	119.81(11)
C(3)-C(2)-C(6)	132.62(11)
C(2)-C(3)-C(4)	107.37(12)
C(5)-C(4)-C(3)	107.08(13)
N(1)-C(5)-C(4)	108.92(12)
O(11)-C(6)-N(7)	122.38(11)
O(11)-C(6)-C(2)	123.58(11)
N(7)-C(6)-C(2)	114.04(10)
C(8)-N(7)-C(6)	126.82(10)
N(10)-C(8)-N(9)	121.10(11)
N(10)-C(8)-N(7)	122.35(11)
N(9)-C(8)-N(7)	116.55(11)
O(13)-C(14)-O(12)	123.85(11)

O(13)-C(14)-C(15)	118.61(11)
O(12)-C(14)-C(15)	117.53(11)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for guanidiniocarbonyl-1H-pyrrole acetate. 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)	46(1)	42(1)	13(1)	1(1)	4(1)
C(2)	33(1)	41(1)	38(1)	10(1)	7(1)	6(1)
C(3)	44(1)	40(1)	47(1)	11(1)	4(1)	5(1)
C(4)	57(1)	45(1)	54(1)	21(1)	9(1)	12(1)
C(5)	49(1)	54(1)	47(1)	21(1)	5(1)	14(1)
C(6)	34(1)	39(1)	41(1)	11(1)	6(1)	2(1)
N(7)	33(1)	34(1)	45(1)	13(1)	2(1)	2(1)
C(8)	34(1)	37(1)	41(1)	12(1)	8(1)	6(1)
N(9)	39(1)	41(1)	52(1)	19(1)	-1(1)	1(1)
N(10)	43(1)	40(1)	63(1)	22(1)	-2(1)	-1(1)
O(11)	47(1)	47(1)	65(1)	22(1)	-9(1)	-10(1)
O(12)	41(1)	35(1)	54(1)	16(1)	1(1)	0(1)
O(13)	42(1)	36(1)	58(1)	11(1)	-2(1)	0(1)
C(14)	38(1)	35(1)	40(1)	11(1)	6(1)	2(1)
C(15)	59(1)	47(1)	62(1)	24(1)	-9(1)	4(1)
O(16)	50(1)	36(1)	69(1)	5(1)	16(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for guanidiniocarbonyl-1H-pyrrole-acetate.

	x	y	z	U(eq)
H(1)	-3840(20)	4030(20)	-5860(20)	56(4)
H(3)	-120(20)	7470(20)	-2950(20)	60(4)
H(4)	-2030(20)	8660(20)	-5090(20)	71(5)
H(5)	-4380(20)	6410(20)	-6790(20)	63(4)
H(7)	895(19)	5421(19)	-1850(19)	51(4)
H(9A)	2900(19)	5100(20)	-3(19)	53(4)
H(9B)	3170(20)	3470(20)	650(20)	70(5)
H(10A)	-520(20)	1620(20)	-1890(20)	65(5)
H(10B)	1100(20)	1380(20)	-530(20)	71(5)
H(15A)	4510(30)	-930(30)	3060(30)	94(6)
H(15B)	5870(30)	630(30)	3730(30)	92(6)
H(15C)	5730(30)	-620(40)	2090(40)	132(10)
H(16A)	2610(20)	-1830(30)	-230(20)	74(5)
H(16B)	6450(30)	2660(20)	1250(20)	86(6)