Anhang 1: Daten der Röntgenstruktur von Methoxycarbonylbiuret

Table 1. Crystal data and structure refinement.

Identification code	BOERN2
Empirical formula	C4 H7 O4 N3 x H2O
Formula weight	179.13
Temperature	293 K
Wavelength	1.5418 A
Crystal system	Triclinic
Space group	P1bar
Unit cell dimensions	a = 4.562(1) A alpha = 76.38(2) deg. b = 8.596(2) A beta = 80.07(2) deg. c = 10.922(3) A gamma = 75.72(2) deg.
Volume	396.1(2) A^3
Z	2
Density (calculated)	1.501 Mg/m^3
Absorption coefficient	12.24 cm^-1
F(000)	188
Crystal size	0.70 x 0.12 x 0.08 mm
Theta range for data collection	4.2 to 58.93 deg.
Index ranges	0<=h<=5, -9<=k<=9, -11<=l<=12
Reflections collected	1306
Independent reflections	1122 [R(int) = .05]
Refinement method	Full-matrix least-squares on F
Data / restraints / parameters	1081 / 0 / 146
Goodness-of-fit on F	3.821
Final R indices [I>2sigma(I)]	R1 = .081, wR2 = .039
R indices (all data)	R1 = .064, wR2 = .042
Absolute structure parameter	0
Extinction coefficient	392(56)
Largest diff. peak and hole	.321 and -.179 e.A^-3

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

	x	y	z	U(eq)
C(1)	1969(5)	7756(3)	6089(2)	38(2)
O(1)	2145(4)	9098(2)	6295(2)	54(2)
N(1)	220(5)	7611(3)	5291(2)	45(2)
N(2)	3661(5)	6326(2)	6757(2)	36(2)
C(2)	3698(5)	4729(3)	6727(2)	33(2)
O(2)	2380(4)	4319(2)	6048(2)	43(2)
N(3)	5464(5)	3534(2)	7550(2)	38(2)
C(3)	7115(5)	3766(3)	8406(2)	38(2)
O(3)	7357(4)	5088(2)	8561(2)	49(2)
O(4)	8406(4)	2295(2)	9035(2)	53(2)
C(4)	10020(1)	2276(5)	10078(3)	65(3)
O(1W)	5851(6)	174(2)	7570(2)	59(2)
H(11)	90(5)	6720(3)	5180(2)	39(7)
H(12)	-780(6)	8700(4)	4810(3)	63(8)
H(2)	4870(5)	6470(3)	7260(3)	50(8)
H(3)	5360(6)	2560(3)	7600(3)	47(8)
H(41)	10760(8)	3290(5)	10020(4)	100(1)
H(42)	11540(8)	1330(5)	10180(4)	110(1)
H(43)	8900(1)	1750(6)	10820(6)	160(2)
H(1W)	7590(9)	-70(5)	7260(5)	120(2)
H(2W)	4550(8)	-220(5)	7270(4)	100(1)

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

C(1)-O(1)	1.238(3)
C(1)-N(1)	1.317(4)
C(1)-N(2)	1.385(3)
N(2)-C(2)	1.362(3)
C(2)-O(2)	1.221(4)
C(2)-N(3)	1.380(3)
N(3)-C(3)	1.373(4)
C(3)-O(3)	1.210(3)
C(3)-O(4)	1.324(3)
O(4)-C(4)	1.455(5)
O(1)-C(1)-N(1)	123.3(2)
O(1)-C(1)-N(2)	117.7(2)
N(1)-C(1)-N(2)	119.1(2)
C(1)-N(2)-C(2)	127.6(2)
N(2)-C(2)-O(2)	124.7(2)
N(2)-C(2)-N(3)	115.4(2)
O(2)-C(2)-N(3)	119.9(2)
C(2)-N(3)-C(3)	127.8(2)
N(3)-C(3)-O(3)	126.0(2)
N(3)-C(3)-O(4)	108.4(2)
O(3)-C(3)-O(4)	125.6(3)
C(3)-O(4)-C(4)	116.9(3)

Table 4. Anisotropic displacement parameters (A^2 x 10^3). 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
C(1)	44(1)	29(1)	43(2)	-8(1)	-14(1)	-8(1)
O(1)	69(1)	28(1)	74(1)	-12(1)	-42(1)	-5(1)
N(1)	58(2)	30(1)	54(1)	-8(1)	-30(1)	-8(1)
N(2)	44(1)	29(1)	40(1)	-8(1)	-21(1)	-7(1)
C(2)	38(1)	29(1)	34(1)	-7(1)	-10(1)	-9(1)
O(2)	56(1)	33(1)	48(1)	-11(1)	-28(1)	-9(1)
N(3)	51(1)	26(1)	43(1)	-6(1)	-23(1)	-7(1)
C(3)	41(1)	38(1)	37(1)	-7(1)	-13(1)	-7(1)
O(3)	66(1)	38(1)	51(1)	-12(1)	-30(1)	-10(1)
O(4)	71(1)	38(1)	55(1)	-3(1)	-39(1)	-6(1)
C(4)	81(3)	69(2)	50(2)	2(2)	-42(2)	-16(2)
O(1W)	68(2)	43(1)	78(2)	-22(1)	-30(1)	-7(1)

Table 5. Torsion angles [deg].

O(1)-C(1)-N(1)-H(11)	-178(2)
O(1)-C(1)-N(1)-H(12)	6(2)
N(2)-C(1)-N(1)-H(11)	0(2)
N(2)-C(1)-N(1)-H(12)	-175(2)
O(1)-C(1)-N(2)-C(2)	176.5(2)
O(1)-C(1)-N(2)-H(2)	-4(2)
N(1)-C(1)-N(2)-C(2)	-2.2(4)
N(1)-C(1)-N(2)-H(2)	178(2)
C(1)-N(2)-C(2)-O(2)	2.8(4)
C(1)-N(2)-C(2)-N(3)	-176.2(2)
H(2)-N(2)-C(2)-O(2)	-177(2)
H(2)-N(2)-C(2)-N(3)	4(2)
N(2)-C(2)-N(3)-C(3)	1.6(3)
N(2)-C(2)-N(3)-H(3)	173(2)
O(2)-C(2)-N(3)-C(3)	-177.6(2)
O(2)-C(2)-N(3)-H(3)	-6(2)
C(2)-N(3)-C(3)-O(3)	-2.0(4)
C(2)-N(3)-C(3)-O(4)	178.1(2)
H(3)-N(3)-C(3)-O(3)	-174(2)
H(3)-N(3)-C(3)-O(4)	6(2)
N(3)-C(3)-O(4)-C(4)	-174.2(2)
O(3)-C(3)-O(4)-C(4)	3.9(4)
C(3)-O(4)-C(4)-H(41)	-24(2)
C(3)-O(4)-C(4)-H(42)	-152(3)
C(3)-O(4)-C(4)-H(43)	115(3)

Table 6. Inter- and Intramolecular Contacts

D-H...A	D...A	D-H	H...A	sym.op. for A
N(1)-H(11)...O(2)	2.975(4)	0.83(3)	2.11(2)	-x,1-y,1-z
N(1)-H(12)...O(1)	2.964(3)	0.98(3)	1.99(3)	-x,2-y,1-z
N(2)-H(2)...O(3)	2.668(3)	0.89(3)	1.95(3)	x,y,z
N(3)-H(3)...O(1W)	2.814(3)	0.83(3)	2.00(3)	x,y,z
O(1W)-H(1W)...O(1)	2.795(4)	0.81(4)	2.19(4)	1+x,-1+y,z
O(1W)-H(2W)...O(1)	2.795(4)	0.89(4)	1.92(5)	x,-1+y,z
N(1)-H(11)...O(2)	2.708 (3)	1.03(3)	2.13(3)	x,y,z

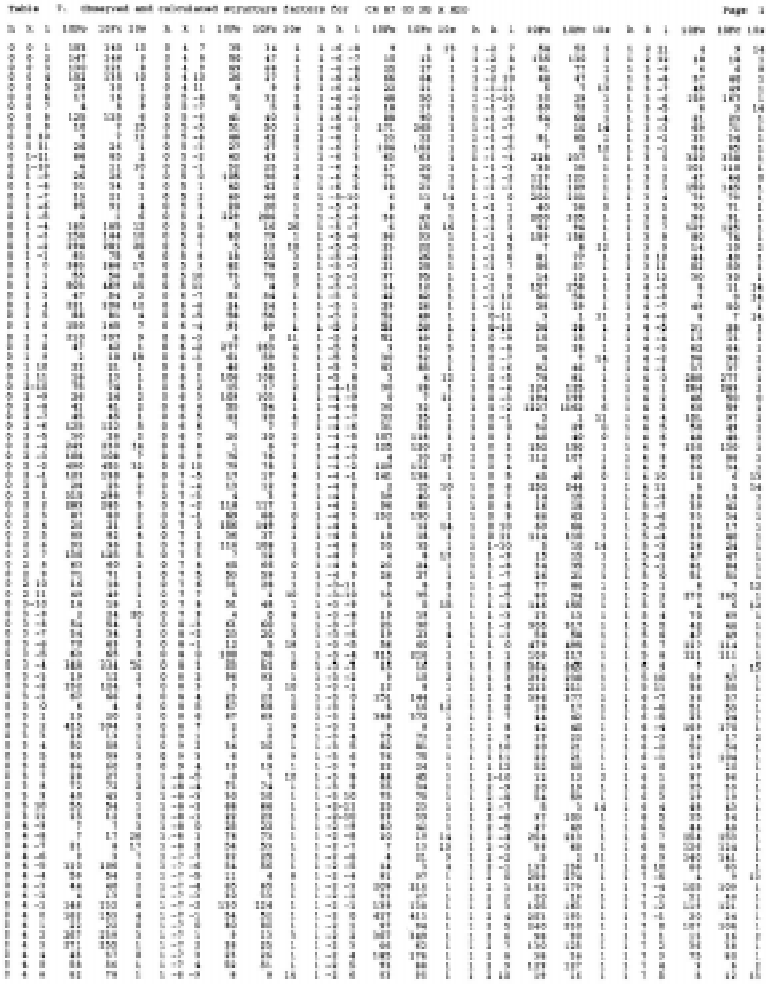

Table 7. Observed and calculated structure factors for [illegible] Page 2

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Table 7. Observed and calculated structure factors for [illegible] Page 3

h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s	h	k	l	10Fo	10Fc	10s
[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Anhang 2: Werte zu Tabelle 95

Verbindung	Nummer	Löslichkeit (g/l)	Stickstoffgehalt der reinen Substanz (%)	Löslichkeit von N (mol/l)
Vergleichssubstanzen				
Harnstoff	1	1080	46.64	36
Isodur gemahlen	2	2	32.16	0.034
Isodur granuliert				
Carbonylharnstoffe				
Triuret	3	0.0025	38.35	0.00007
Tetrauret	4	0.034	37.03	0.0009
Pentauret	5	0.003	36.2	0.00008
Hexauret	6	0	35.63	0.000001
Alkoxycarbonylharnstoffe				
Methoxycarbonylharnstoff	7	0.12	23.72	0.002
Ethoxycarbonylharnstoff	8	0.08	21.1	0.0012
Methoxycarbonylbiuret	9	0.068	27.1	0.0013
Ethoxycarbonylbiuret	10	0.032	23.99	0.0005
Methoxycarbonyltriuret	11	0.007	27.45	0.00003
Ethoxycarbonyltriuret	12	0.003	25.68	0.00006
Methoxycarbonyltetrauret	13	0	28.33	0.000001
Ethoxycarbonyltetrauret	14	0	26.81	0.000001
Harnstoffderivate				
Acetylharnstoff + 5% Harnstoff	15	52.6	27.44	1
Propylharnstoff	16	395	27.7	7.7
tert. Butylharnstoff	17	20.8	23.9	0.36
N-Methoxyharnstoff	18		31.1	
Bis 1,1-methylendiharnstoff MH23	19	25.3	42.4	0.77
Bis 1,2-ethyldiureid	20	72.5	38.22	1.98
Bis 1,3-propyldiureid	21	77.4	34.98	1.93
Bis 1,4-butyldiureid	22	0.117	32.16	0.003
Bis 1,5-pentyldiureid	23	0.019	29.76	0.0004
Bis 1,6-hexyldiureid	24	0.036	27.7	0.0007
Biuretderivate				
1-Methylbiuret	25	59	35.88	1.51
1-Ethylbiuret	26	86	32.1	1.98
1-Propylbiuret	27	10.9	28.95	0.23

Verbindung	Nummer	Löslichkeit (g/l)	Stickstoffgehalt der reinen Substanz (%)	Löslichkeit von N (mol/l)
Biuretderivate				
Acetylbiuret	29	8.3	28.96	0.17
Diacetylbiuret	30	7.2	22.45	0.12
1,1-Dimethylbiuret	31	57	32.04	1.31
1,3-Dimethylbiuret	32	211.6	32.04	4.83
Ethylendibiuret	33	0	36.19	0.000001
1,1-Diethylbiuret	34	14.4	26.4	2.73
Triuretderivate				
3-Methyltriuret	35	0.023	34.99	0.00058
3-Ethyltriuret	36	1.2	32.2	0.021
3-Methoxytriuret	37	3.25	31.81	0.074
1,1 Dimethyltriuret	38	6.7	32.2	0.117
Sonstige untersuchte Verbindungen				
Biscarbamoylpiperazin	39	3.66	32.54	0.085
Carbamidsäureanhydrid	40	51.3	21.54	0.78
Acetylendiharnstoff	41	0.84	39.42	0.0237
Oxaldiamid	42		31.8	0.01
Malondiamid	43		27.5	3.58
Succindiamid	44		24.1	0.1