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Three-Dimensional X-ray Analysis of the Complex $CaBr_2.10H_2O.2(CH_2)_6N_4$

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Crystals of the complex $CaBr_2.10H_2O.2(CH_2)_6H_4$ are triclinic, space group $P\bar{1}$, with $a=9{\cdot}89\pm0{\cdot}02$, $b=9{\cdot}75\pm0{\cdot}02$, $c=9{\cdot}58\pm0{\cdot}02$, $\alpha=94°29'\pm12'$, $\beta=100°39'\pm12'$, $\gamma=119°20'\pm12'$, $Z=1$. The crystal structure has been determined by the heavy-atom method and then refined by three-dimensional Fourier synthesis and several cycles of differential synthesis. The structure is characterized by layers parallel to (001), in which each hexamethylentetramine molecule links three different $Ca(H_2O)_6^{2+}$ octahedra and each $Ca(H_2O)_6^{2+}$ octahedron links six different hexamethylenetetramine molecules. The structure is fully hydrogen bonded.

Introduction

The problem of solvation of biological macromolecules in aqueous solutions has become extremely interesting within the past few years and an increasing number of studies on simple models have been carried out.

It appeared of some interest to us to clarify some structural aspects of complexes between organic bases and inorganic salts in which high forms of hydration are often stabilized. Hexamethylenetetramine (HMT) forms a large series of complexes with different inorganic salts, linking also a high number of water molecules (Table 1). These complexes were first crystallized by Barbieri & Calzolari (1910). Bertinotti & Liquori (1953) investigated the structure of the complex $CaBr_2.10H_2O.2$(HMT) and of the corresponding magnesium chloride complex by two-dimensional X-ray analysis. However, the many superpositions of atoms made it impossible to unravel the structures completely. It was therefore decided to carry out a three-dimensional analysis of the complex $CaBr_2.10H_2O.2$(HMT) and to examine the relationship between this structure and that of a cubic modification studied by Addamiano & Giacomello (1951). Some preliminary results have already been reported (De Santis, Kovacs, Liquori & Mazzarella, 1965).

Table 1. *Some complexes between hexamethylenetetramine and inorganic salts*

General formula	A
A . $10H_2O$. 2(HMT)	$CaBr_2$, $MgCl_2$, $MnCl_2$, $CoCl_2$, $NiCl_2$, $MnBr_2$, $MgBr_2$, $CoBr_2$, $NiBr_2$, NiI_2, CoI_2, MnI_2, MgI_2, $Mg(SCN)_2$, $Mg(NO_3)_2$, $Co(NO_3)_2$, $Mn(NO_3)_2$, $Y(NO_3)_3$.
A . $8H_2O$. 2(HMT)	$Mg(ClO_4)_2$, $Co(ClO_4)_2$, $Ni(ClO_4)_2$.
A . $7H_2O$. 2(HMT)	$MnCr_2O_7$, $MgCr_2O_7$.

Table 2. *Observed* ($F_o \times 10$) *and calculated* ($F_c \times 10$) *structure factors*

H	K	L	FO	FC
1	0	0	155	-193
2	0	0	38	-29
3	0	0	427	-415
4	0	0	271	313
5	0	0	343	395
6	0	0	253	266
0	1	0	355	-389
1	1	0	134	91
2	1	0	476	434
-2	1	0	869	827
3	1	0	623	611
-3	1	0	220	217
4	1	0	350	314
-4	1	0	152	-154
6	1	0	113	-86
-6	1	0	24	-33
7	1	0	169	161
-7	1	0	267	268
8	1	0	159	161
-8	1	0	159	158
-9	1	0	17	12
0	2	0	43	16
1	2	0	607	659
-1	2	0	355	332
2	2	0	63	62
-2	2	0	959	-883
3	2	0	218	-231
-3	2	0	26	-15
4	2	0	288	-283
-4	2	0	171	-114
5	2	0	147	169
-5	2	0	808	755
6	2	0	259	267
-6	2	0	203	157
7	2	0	105	87
-7	2	0	154	-163
-8	2	0	166	-177
-9	2	0	89	104
-10	2	0	108	115
-11	2	0	50	51
0	3	0	372	-426
1	3	0	68	26
-1	3	0	581	608
2	3	0	54	-60
-2	3	0	504	474
3	3	0	194	205
-3	3	0	56	48
4	3	0	204	172
-4	3	0	155	-147
5	3	0	12	-28
-5	3	0	91	-82
-6	3	0	82	79
-7	3	0	346	325
-8	3	0	154	134
-9	3	0	98	-92
-10	3	0	56	-48
-11	3	0	38	40
0	4	0	295	280
1	4	0	423	413
-1	4	0	197	-202
2	4	0	273	280
-2	4	0	701	-580
3	4	0	36	-36
-3	4	0	194	281
4	4	0	99	-104
-4	4	0	747	731
5	4	0	14	-12
-5	4	0	73	-48
6	4	0	77	60
-6	4	0	98	90
7	4	0	131	96
-7	4	0	169	-137
-8	4	0	110	95
-9	4	0	166	156
-10	4	0	105	106
-11	4	0	80	77
-12	4	0	17	11
0	5	0	392	421
1	5	0	61	-57
-1	5	0	59	52
2	5	0	115	-116
-2	5	0	364	385
3	5	0	61	60
-3	5	0	185	-200
4	5	0	196	182
-4	5	0	85	73
5	5	0	108	99
-5	5	0	183	180
-6	5	0	343	447
-7	5	0	206	168
-8	5	0	94	88
-9	5	0	40	-54
-10	5	0	42	39
-11	5	0	129	104
-12	5	0	64	57
0	6	0	101	-81
1	6	0	105	109
-1	6	0	73	-62
2	6	0	308	312
-2	6	0	246	237
3	6	0	117	128
-3	6	0	311	302
-4	6	0	341	344
-5	6	0	115	103
-6	6	0	10	-2
-7	6	0	80	-63
-8	6	0	115	92
-9	6	0	211	188
-10	6	0	54	62
-11	6	0	43	-45
0	7	0	162	174
1	7	0	63	62
-1	7	0	204	197
-2	7	0	52	-43
-3	7	0	57	-62
-4	7	0	190	-190
-5	7	0	462	430
-6	7	0	24	-4
-7	7	0	52	56
-8	7	0	145	-125
-9	7	0	49	-31
-10	7	0	77	62
-11	7	0	122	98
-12	7	0	29	28
0	8	0	99	-104
1	8	0	47	24
-1	8	0	57	-62
2	8	0	106	102
-2	8	0	84	80
-3	8	0	215	210
-4	8	0	112	109
-5	8	0	162	-150
-6	8	0	140	-166
-7	8	0	180	234
-8	8	0	63	73
-9	8	0	57	73
-10	8	0	12	-5
-11	8	0	12	0
-12	8	0	49	48
0	9	0	120	111
1	9	0	63	54
-1	9	0	22	10
-2	9	0	57	-48
-3	9	0	12	5
-4	9	0	147	139
-5	9	0	101	93
-6	9	0	189	196
-7	9	0	87	-103
-8	9	0	35	24
-9	9	0	31	21
-10	9	0	138	121
-11	9	0	70	74
-12	9	0	7	21
1	10	0	12	10
-1	10	0	75	68
-2	10	0	103	106
-3	10	0	78	63
-6	10	0	70	48
-5	11	0	75	80
-6	11	0	54	55
0	0	1	271	298
1	0	1	278	288
-1	0	1	84	68
2	0	1	752	782
-2	0	1	549	-563
3	0	1	288	275
-3	0	1	197	271
4	0	1	182	-213
-4	0	1	582	675
5	0	1	110	-125
-5	0	1	227	241
6	0	1	105	108
-6	0	1	85	-76
7	0	1	218	236
-7	0	1	80	-85
8	0	1	122	158
-8	0	1	98	142
-9	0	1	106	165
-10	0	1	31	52
0	1	1	861	1070
0	-1	1	138	-160
1	1	1	36	27
-1	1	1	360	259
1	-1	1	360	356
1	1	-1	931	892
2	1	1	322	-286
-2	1	1	423	340
2	-1	1	386	-394
2	1	-1	642	579
3	1	1	103	113
-3	1	1	248	-256
3	-1	1	168	192
3	1	-1	266	-244
4	1	1	189	187
-4	1	1	91	-82
4	-1	1	414	394
4	1	-1	197	-186
5	1	1	297	290
-5	1	1	603	542
5	-1	1	180	173
5	1	-1	52	-23
6	1	1	103	88
-6	1	1	287	280
6	-1	1	164	-126
6	1	-1	343	302
7	1	1	19	5
-7	1	1	259	283
7	-1	1	112	-93
7	1	-1	206	180
8	1	1	17	-25
-8	1	1	120	-115
8	-1	1	17	20
-9	1	1	59	-66
9	-1	1	99	97
-10	1	1	15	39
10	-1	1	85	73
-11	1	1	106	92
0	2	1	218	-265
0	-2	1	491	450
1	2	1	350	344
-1	2	1	343	-357
1	-2	1	574	840
1	2	-1	521	-506
2	2	1	686	670
-2	2	1	540	601
2	-2	1	318	281
2	2	-1	428	-404
3	2	1	341	352
-3	2	1	750	738
3	-2	1	901	-898
3	2	-1	162	168
4	2	1	84	-79
-4	2	1	141	135
4	-2	1	399	-395
4	2	-1	329	328
5	2	1	105	-98
-5	2	1	217	-182
5	-2	1	110	118
5	2	-1	117	101
6	2	1	14	-4
-6	2	1	80	-107
6	-2	1	386	342
6	2	-1	136	131
7	2	1	120	122
-7	2	1	183	171
7	-2	1	132	151
7	2	-1	171	-153
-8	2	1	36	-26
8	-2	1	26	-31
-9	2	1	152	155
9	-2	1	12	-13
-10	2	1	10	[illegible]
-11	2	1	7	-13
11	-2	1	38	46
0	3	1	518	588
0	-3	1	528	-423
1	3	1	381	367
-1	3	1	392	-339
1	-3	1	337	-352
1	3	-1	300	357
2	3	1	8	-22
-2	3	1	259	-260
2	-3	1	45	45
2	3	-1	381	394
3	3	1	215	-218
-3	3	1	533	-471
3	-3	1	344	359
3	3	-1	134	109
4	3	1	78	69
-4	3	1	59	69
4	-3	1	745	702
4	3	-1	239	-228
5	3	1	157	161
-5	3	1	383	429
5	-3	1	231	-235
5	3	-1	143	-148
6	3	1	154	161
-6	3	1	217	212
6	-3	1	31	12
6	3	-1	71	53
-7	3	1	155	-198
7	-3	1	56	57
7	3	-1	206	212
-8	3	1	68	-63
8	-3	1	194	188
-9	3	1	35	-47
9	-3	1	154	149
-10	3	1	112	123
10	-3	1	10	35
-11	3	1	77	71
11	-3	1	8	2
-12	3	1	36	48
0	4	1	474	-481
0	-4	1	672	705
1	4	1	155	-166
-1	4	1	288	283
1	-4	1	444	462
1	4	-1	329	321
2	4	1	117	114
-2	4	1	78	105
2	4	-1	334	-322
3	4	1	232	251
-3	4	1	250	283
3	-4	1	94	78
3	4	-1	49	-40
4	4	1	148	136
-4	4	1	241	227
4	-4	1	185	-167
4	4	-1	56	41
5	4	1	87	-87
-5	4	1	203	-203
5	-4	1	386	404
5	4	-1	299	304
6	4	1	71	-78
-6	4	1	35	-42
6	-4	1	481	513
-7	4	1	175	205
7	-4	1	150	156
-8	4	1	280	290
8	-4	1	94	-88
-9	4	1	14	10
9	-4	1	66	-60
-10	4	1	12	-20
10	-4	1	70	71
-11	4	1	10	-8
11	-4	1	161	151
-12	4	1	120	113
0	5	1	302	300
0	-5	1	91	-105
1	5	1	274	259
-1	5	1	136	124
1	-5	1	68	-78
1	5	-1	173	179
2	5	1	43	49
-2	5	1	416	-422
2	-5	1	418	366
2	5	-1	353	373
3	5	1	47	-61
-3	5	1	267	284
3	-5	1	411	392
3	5	-1	124	127
4	5	1	14	-6
-4	5	1	353	410
4	-5	1	161	158
4	5	-1	80	75
-5	5	1	509	520
5	-5	1	22	-20
-6	5	1	92	89
6	-5	1	245	-206
-7	5	1	155	-168
7	-5	1	189	182
7	5	-1	70	66
-8	5	1	36	-12
8	-5	1	239	234
-9	5	1	157	152
9	-5	1	112	97
-10	5	1	159	154
10	-5	1	33	-15
-11	5	1	133	136
11	-5	1	47	-36
-12	5	1	42	-40
12	-5	1	38	30
0	6	1	14	-23
0	-6	1	437	444
1	6	1	103	-87
-1	6	1	152	163
1	-6	1	124	119
1	6	-1	22	-16
2	6	1	119	117
-2	6	1	516	492
2	-6	1	274	-252
2	6	-1	119	122
3	6	1	138	141
-3	6	1	39	100
3	-6	1	280	-238
3	6	-1	80	-70
4	6	1	73	80
-4	6	1	71	-84
4	-6	1	117	110
-5	6	1	145	-147
5	-6	1	430	467
-6	6	1	199	223
6	-6	1	196	187
6	6	-1	103	84
-7	6	1	285	266
7	-6	1	134	-114
-8	6	1	59	[illegible]
8	-6	1	89	-77
-10	6	1	15	32
10	-6	1	141	113
-11	6	1	89	56
11	-6	1	70	50
-12	6	1	66	44
12	-6	1	26	38
0	7	1	49	38
0	-7	1	73	-71
1	7	1	140	133
-1	7	1	140	-134
1	-7	1	101	70
1	7	-1	22	-44
2	7	1	80	95
-2	7	1	10	9
2	-7	1	252	241
2	7	-1	31	27
-3	7	1	136	155
3	-7	1	105	84
3	7	-1	122	143
-4	7	1	217	221
4	7	-1	61	60
-5	7	1	143	143
5	-7	1	22	-39
-6	7	1	50	54
6	-7	1	47	-50
-7	7	1	136	-157
7	-7	1	213	206
-8	7	1	89	62
8	-7	1	89	81
-9	7	1	171	180
9	-7	1	26	-8
-10	7	1	89	93
10	-7	1	26	-27
-11	7	1	12	21
11	-7	1	10	-7
-12	7	1	28	-21
12	-7	1	57	46
0	8	1	68	64
1	8	1	22	4
-1	8	1	89	94
1	-8	1	29	-33
1	8	-1	189	192
-2	8	1	120	120
2	-8	1	113	-133
2	8	-1	47	56
-3	8	1	12	2
3	-8	1	115	110
3	8	-1	49	-6
4	8	1	64	65
-4	8	1	12	3
4	-8	1	208	168
-5	8	1	129	106
5	-8	1	1	14
-6	8	1	29	-27
6	-8	1	133	142
-7	8	1	145	179
7	-8	1	96	-93
-8	8	1	33	37
8	-8	1	66	-56
-9	8	1	68	-63
9	-8	1	91	81
-10	8	1	12	-7
10	-8	1	138	110
11	-8	1	71	75
-11	8	1	63	42
-12	8	1	77	80
1	9	1	17	16
-1	9	1	14	-17
1	-9	1	80	93
1	9	-1	40	45
-2	9	1	14	38
2	-9	1	110	121
-3	9	1	98	101
3	-9	1	5	22
-4	9	1	117	134
4	-9	1	56	-59
-5	9	1	35	-33
5	-9	1	64	52
-6	9	1	105	-96
6	-9	1	157	137
-7	9	1	12	22
7	-9	1	105	108
-8	9	1	52	47
8	-9	1	94	99
-9	9	1	87	111
9	-9	1	10	-3
-10	9	1	12	34
10	-9	1	42	32
-11	9	1	10	-2
11	-9	1	92	68
-12	9	1	28	28
0	10	1	36	31
1	10	1	8	18
-1	10	1	70	73
1	-10	1	19	10
1	10	-1	47	52
3	-10	1	89	89
4	-10	1	211	206
-5	10	1	108	83
5	-10	1	85	68
-6	10	1	113	86
6	-10	1	45	-23
-7	10	1	31	37
-2	11	1	57	65
2	-11	1	63	57
-3	11	1	84	81
5	-11	1	98	81
-6	11	1	75	67
6	-11	1	71	72
-7	11	1	64	50
-6	12	1	59	44
7	-12	1	61	42
0	0	2	642	-695
1	0	2	453	-463
-1	0	2	768	834
2	0	2	[illegible]	15
-2	0	2	628	647
3	0	2	525	543
-3	0	2	133	112
4	0	2	178	183
-4	0	2	42	-65
5	0	2	47	-59
-5	0	2	12	7
6	0	2	206	-247
-6	0	2	255	274
7	0	2	66	76
-7	0	2	133	154
8	0	2	63	83
-8	0	2	105	145
9	0	2	80	93
-9	0	2	15	20
0	1	2	577	505
0	-1	2	437	441
1	1	2	889	801
-1	1	2	262	-284
1	-1	2	675	758
1	1	-2	271	-207
2	1	2	778	623
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4	-6	4	236	223
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2	7	-4	61	43
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3	-7	4	117	133
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5	-7	4	162	-166
-6	7	4	94	91
6	-7	4	183	175
-7	7	4	14	-6
7	-7	4	194	192
-8	7	4	119	121
8	-7	4	143	137
-9	7	4	92	84
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Table 2 (*cont.*)

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2	-8	4	92	-109
2	8	-4	64	63
-3	8	4	17	-9
3	-8	4	68	83
-4	8	4	35	-38
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6	-8	4	12	20
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7	-8	4	119	-124
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8	-8	4	57	54
-9	8	4	12	-28
9	-8	4	119	115
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10	-8	4	82	68
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4	-9	4	140	-145
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5	-9	4	56	51
-6	9	4	43	-40
6	-9	4	82	87
-7	9	4	61	62
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8	-9	4	10	8
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9	-9	4	10	-16
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10	-9	4	35	-23
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1	-10	4	73	-71
2	-10	4	52	58
3	-10	4	70	63
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1	2	-5	7	2
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H	K	L	FO	FC
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4	2	5	140	126
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4	-2	5	115	100
4	2	-5	152	128
5	2	5	49	46
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5	-2	5	225	-218
5	2	-5	78	-77
6	2	5	10	25
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6	-2	5	12	18
6	2	-5	75	-74
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-7	2	5	171	147
7	-2	5	101	106
7	2	-5	77	70
-8	2	5	234	217
8	-2	5	91	95
-9	2	5	24	-28
9	-2	5	7	27
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7	-5	5	106	-105

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3	-11	5	61	76
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7	-11	5	80	83
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3	4	-6	101	103
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Table 2 (*cont.*)

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7	1	-9	28	22
-8	1	9	89	100
-9	1	9	47	64
0	2	9	98	108
0	-2	9	64	57
1	2	9	10	37
-1	2	9	29	25
1	-2	9	[illegible]	-56
1	2	-9	145	149
2	2	9	8	20
-2	2	9	12	12
2	-2	9	54	-55
2	2	-9	85	86
3	2	9	40	-36
-3	2	9	57	-75
3	-2	9	10	20
3	2	-9	89	-84
-4	2	9	78	84
4	-2	9	94	91
4	2	-9	43	-48
-5	2	9	106	135
5	-2	9	80	72
-6	2	9	73	72
6	2	-9	40	46
7	2	-9	154	121
0	3	9	10	-7
0	-3	9	103	101
1	3	9	8	25
-1	3	9	12	8
1	-3	9	124	118
1	3	-9	75	-80
2	3	9	54	35
-2	3	9	70	72
2	-3	9	145	150
-3	3	9	68	65
3	-3	9	61	-56
-4	3	9	89	89
4	-3	9	10	-3
4	3	-9	94	107
-5	3	9	89	-94
5	-3	9	35	-27
5	3	-9	89	92
-6	3	9	12	22
6	-3	9	117	104
-7	3	9	64	65
7	3	-9	66	-6
-8		9	29	36
-9	3	9	8	22
0	4	9	10	-7
0	-4	9	68	-66
1	4	9	75	66
-1	4	9	45	51
1	-4	9	12	-16
1	4	-9	122	126
-2	4	9	66	-68
2	-4	9	12	20
2	4	-9	180	193
-3	4	9	29	48
3	-4	9	110	114
3	4	-9	52	52
-4	4	9	29	31
4	-4	9	94	91
4	4	-9	12	-20
-5	4	9	96	99
5	-4	9	10	-3
5	4	-9	66	-76
6	4	-9	89	75
-9	4	9	54	53
-10	4	9	50	64
0	5	9	7	13
0	-5	9	245	183
1	5	9	7	-11
-1	5	9	49	42
1	-5	9	148	149
1	5	-9	33	31
-2	5	9	35	24
2	-5	9	66	-67
2	5	-9	56	-62
-3	5	9	56	43
3	-5	9	31	-11
3	5	-9	10	-20
-4	5	9	12	-9
4	-5	9	33	-25
4	5	-9	87	80
-5	5	9	57	57
5	-5	9	101	94
5	5	-9	89	94
-6	5	9	12	20
6	-5	9	61	48
-7	5	9	47	50
-8	5	9	10	15
-9	5	9	63	54
0	6	9	0	24
0	-6	9	82	-76
-1	6	9	12	-32
1	-6	9	49	-37
1	6	-9	38	34
-2	6	9	71	57
2	-6	9	99	100
2	6	-9	92	72
-3	6	9	40	27
3	-6	9	117	108
3	6	-9	127	117
-4	6	9	75	73
4	-6	9	14	24
-5	6	9	14	24
5	-6	9	38	-23
-6	6	9	12	14
6	-6	9	43	-38
-8	6	9	85	68
0	-7	9	115	113
1	-7	9	10	22
1	7	-9	82	80
2	-7	9	52	-58
2	7	-9	8	-11
3	-7	9	84	-64
-4	7	9	8	17
4	-7	9	49	44
-5	7	9	8	13
5	-7	9	92	90
-6	7	9	8	23
6	-7	9	57	49
-7	7	9	33	33
0	-8	9	64	-49
1	-8	9	10	17
1	8	-9	56	-43
2	-8	9	145	148
5	-8	9	47	-42
0	-9	9	3	65
2	-9	9	49	-63
4	-9	9	89	104
0	0	10	40	47
1	0	10	40	58
-1	0	10	56	-50
2	0	10	56	67
-2	0	10	15	-16
-4	0	10	92	117
-5	0	10	84	83
0	1	10	15	20
0	-1	10	17	-10
1	1	-10	73	57
2	1	10	10	-7
-2	1	10	63	69
2	-1	10	14	33
2	1	-10	91	85
-3	1	10	17	20
3	-1	10	43	50
3	1	-10	54	50
-4	1	10	17	-10
4	-1	10	57	60
4	1	-10	15	-24
-5	1	10	15	21
-6	1	10	82	91
-7	1	10	73	67
7	1	-10	115	89
0	2	10	8	-12
0	-2	10	110	105
1	2	10	80	71
-1	2	10	10	-2
1	-2	10	112	105
1	2	-10	42	35
2	2	10	21	18
-2	2	10	10	1
2	-2	10	10	-1
2	2	-10	106	-88
-3	2	10	103	109
3	-2	10	61	-52
3	2	-10	38	-40
-4	2	10	54	54
4	-2	10	31	28
4	2	-10	66	64
-5	2	10	78	67
5	2	-10	154	131
-6	2	10	33	-37
6	2	-10	43	42
7	2	-10	64	-55
0	3	10	70	72
0	-3	10	113	-89
1	3	10	12	-4
-1	3	10	8	18
1	-3	10	10	22
1	3	-10	10	23
-2	3	10	33	18
2	-3	10	66	68
2	3	-10	119	103
-3	3	10	10	-16
3	-3	10	119	111
3	3	-10	136	123
-4	3	10	28	32
4	-3	10	8	5
-5	3	10	36	47
5	3	-10	85	-78
-6	3	10	38	37
6	3	-10	50	44
-1	4	10	8	-17
1	-4	10	77	72
1	4	-10	94	81
-2	4	10	68	68
2	-4	10	33	-39
2	4	-10	10	-4
-3	4	10	35	38
3	-4	10	10	-24
3	4	-10	59	-64
-4	4	10	68	57
4	-4	10	8	12
-5	4	10	10	-24
5	-4	10	94	103
5	4	-10	85	81
-8	4	10	57	51
0	-5	10	10	-7
-1	5	10	7	58
1	5	-10	57	-48
2	-5	10	134	125
2	5	-10	70	48
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3	-5	10	78	56
3	5	-10	106	96
-4	5	10	26	25
4	-5	10	7	-9
-5	5	10	47	45
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-6	5	10	36	34
0	-6	10	80	68
1	-6	10	47	-30
1	6	-10	115	105
2	-6	10	54	-55
2	6	-10	38	34
3	-6	10	12	-9
3	6	-10	94	-48
4	-6	10	78	72
0	-7	10	8	6
1	-7	10	92	86
1	7	-10	49	-50
2	-7	10	61	61
3	-7	10	8	12
4	-7	10	40	-46
-2	0	11	40	52
-3	0	11	103	105
0	1	11	36	26
0	-1	11	70	73
-1	1	11	15	21
1	-1	11	10	13
1	1	-11	64	5
2	1	11	36	-47
3	1	-11	14	-11
-4	1	11	38	56
-5	1	11	78	74
5	1	-11	63	69
6	1	-11	54	56
0	2	11	7	-7
0	-2	11	29	-0
-1	2	11	64	31
1	-2	11	7	15
1	2	-11	38	-41
-2	2	11	61	67
2	-2	11	73	75
2	2	-11	63	60
-3	2	11	8	27
3	2	-11	47	46
4	2	-11	119	100
-7	2	11	57	50
0	-3	11	91	72
-1	3	11	5	1
1	-3	11	8	-5
1	3	-11	71	69
-2	3	11	7	5
2	3	-11	75	62
-3	3	11	8	7
-4	3	11	89	91
1	-4	11	126	107
1	4	-11	8	-36
2	-4	11	45	44
2	4	-11	8	-25
3	4	-11	75	71
4	4	-11	57	73
0	-5	11	7	-2
1	-5	11	56	-38
1	5	-11	78	80
2	-5	11	26	-26
2	5	-11	70	66
0	-6	11	66	61
1	-6	11	78	71
2	-6	11	31	37
1	2	-12	31	39
2	2	-12	36	34

Table 3. *Final fractional atomic coordinates and their standard deviations* (Å)

	x	y	z	σ_x	σ_y	σ_z
C(1)	0·2138	0·5721	0·1204	0·009	0·008	0·008
C(2)	0·3200	0·7807	0·3318	0·008	0·008	0·007
C(3)	0·3990	0·5867	0·3301	0·008	0·007	0·007
C(4)	0·3990	0·8410	0·1107	0·009	0·007	0·008
C(5)	0·4852	0·6515	0·1118	0·008	0·008	0·006
C(6)	0·5857	0·8585	0·3234	0·008	0·009	0·008
N(1)	0·2631	0·7406	0·1708	0·005	0·006	0·005
N(2)	0·3501	0·5448	0·1706	0·006	0·006	0·006
N(3)	0·4552	0·7574	0·3859	0·007	0·007	0·006
N(4)	0·5386	0·8215	0·1602	0·006	0·006	0·005
O(1)	0·0220	0·8214	0·1346	0·006	0·007	0·007
O(2)	0·2461	0·2170	0·1344	0·006	0·006	0·007
O(3)	0·1567	0·9499	0·8720	0·006	0·006	0·006
O(4)	0·0650	0·6993	0·6582	0·015	0·012	0·011
O(5)	0·4954	0·2081	0·3058	0·007	0·007	0·006
Ca	0·0000	0·0000	0·0000	0·000	0·000	0·000
Br	0·1878	0·4389	0·6794	0·001	0·001	0·001

Table 4. *Final temperature factor coefficients*

The coefficients are the values of b_{ij} in the expression $\exp\,[-(b_{11}h^2+b_{12}hk^2+b_{13}hl+b_{22}k^2+b_{23}kl+b_{33}l^2)]$

	b_{11}	b_{12}	b_{13}	b_{22}	b_{23}	b_{33}
C(1)	0·0104	0·0108	0·0030	0·0129	0·0048	0·0131
C(2)	0·0151	0·0142	0·0132	0·0134	0·0062	0·0113
C(3)	0·0173	0·0164	0·0041	0·0110	0·0063	0·0110
C(4)	0·0137	0·0164	0·0142	0·0130	0·0115	0·0147
C(5)	0·0134	0·0159	0·0092	0·0156	0·0004	0·0120
C(6)	0·0138	0·0126	0·0057	0·0156	0·0028	0·0116
N(1)	0·0095	0·0137	0·0086	0·0142	0·0073	0·0122
N(2)	0·0117	0·0133	0·0061	0·0107	0·0065	0·0123
N(3)	0·0142	0·0130	0·0053	0·0126	0·0040	0·0092
N(4)	0·0114	0·0114	0·0076	0·0133	0·0030	0·0091
O(1)	0·0138	0·0212	0·0181	0·0185	0·0235	0·0214
O(2)	0·0133	0·0132	−0·0015	0·0127	0·0019	0·0179
O(3)	0·0132	0·0113	0·0155	0·0142	0·0008	0·0163
O(4)	0·0430	0·0500	0·0000	0·0290	−0·0065	0·0240
O(5)	0·0150	0·0145	0·0008	0·0173	0·0030	0·0107
Ca	0·0081	0·0099	0·0061	0·0093	0·0053	0·0103
Br	0·0164	0·0164	0·0102	0·0207	0·0182	0·0166

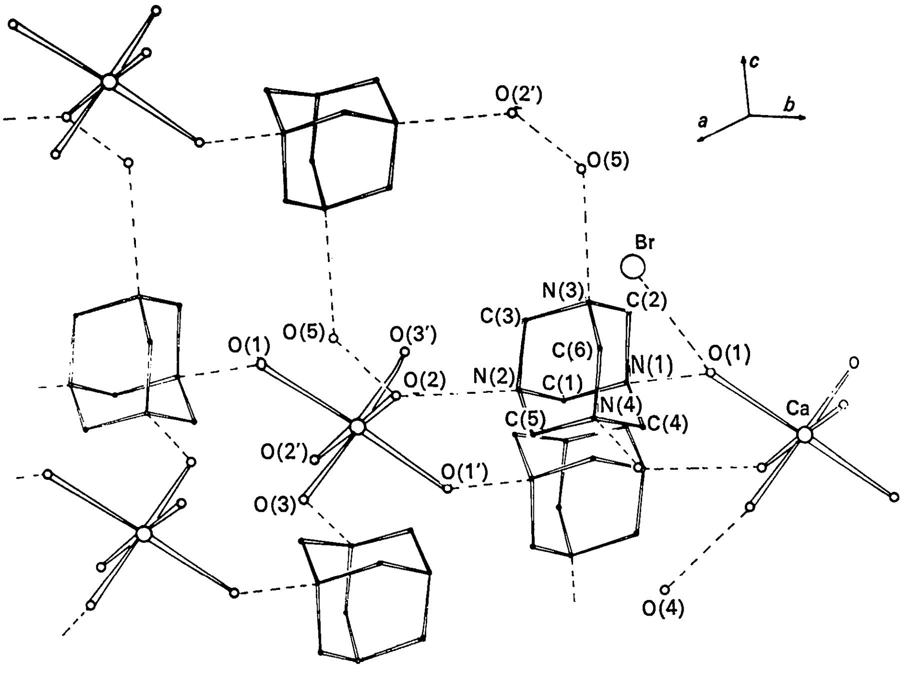

Fig. 1. Perspective view of the structure.

Experimental

Crystals of the complex $CaBr_2.10H_2O.2(HMT)$ were grown from an aqueous solution in which HMT and $CaBr_2$ were in a stoichiometric ratio. If the crystallization temperature is kept above 20 °C, the cubic form studied by Addamiano & Giacomello (1951) with two-dimensional X-ray data is obtained. Lowering the crystallization temperature yields a triclinic form which is common to most of the compounds in the series. The crystals grow as platelets with pseudo-hexagonal symmetry. Large well developed specimens were cut to plates of approximately $0{\cdot}2 \times 0{\cdot}2 \times 0{\cdot}1$ mm perpendicular to the crystal directions [100], [010] and [001]. At room temperature the triclinic crystals are affected by the presence even of traces of water, and the lattice becomes disordered; they were therefore dried before the temperature was raised, and mounted in a sealed Lindemann capillary.

The multi-film equi-inclination photographic method with Ni-filtered Cu $K\alpha$ radiation was used for collecting intensity data. Seventeen layers perpendicular to [100] and [010] axes were recorded, including 2824 independent reflexions with intensities above the background of the 3560 in the limiting sphere of Cu $K\alpha$ radiation. The intensities were estimated by comparison with a calibrated film strip and were corrected for the Lorentz–polarization factor by a computer program which includes the Phillips (1954) spot-shape correction in non-zero layer photographs. No absorption correction was applied. The best scale constant was found for every layer by using the least-squares method described by Rollett & Sparks (1960).

Crystal data

$CaBr_2.10H_2O.2(HMT)$ is triclinic with

$a = 9{\cdot}89 \pm 0{\cdot}02$ Å	$\alpha = 94°29' \pm 12'$
$b = 9{\cdot}75 \pm 0{\cdot}02$	$\beta = 100°39' \pm 12'$
$c = 9{\cdot}58 \pm 0{\cdot}02$	$\gamma = 119°20' \pm 12'$

$D_x = 1{\cdot}41$ g.cm^{-3}

Space group $P\bar{1}$

$Z = 1$

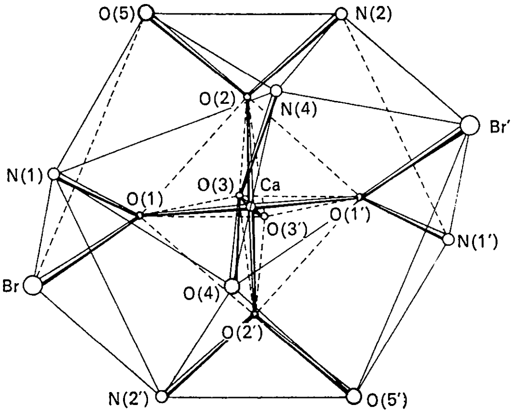

Fig. 2. Environment of the calcium ion.

The measured density of $1{\cdot}44$ g.cm^{-3} is slightly larger than the calculated density. This effect is probably due to the tendency of the crystals to transform into a monometric form which has an experimental density of $1{\cdot}46$ g.cm^{-3}. The space group can be taken as $P\bar{1}$, since the chemical unit is consistent with a centrosymmetric distribution of atoms. The calcium atom is therefore at the centre of symmetry.

Determination and refinement of the structure

In order to determine the bromine position a three-dimensional Patterson function was calculated, which clearly shows a Br–Br and a Ca–Br vector. The collinearity of these two vectors confirms the centrosymmetry of the $CaBr_2$ group. This enabled us to fix the coordinates of the bromine atoms. A three-dimensional heavy atom Fourier synthesis, in which the signs were derived from the positions of Ca^{2+} and Br^-, shows, well above the background, fifteen peaks corresponding to the other atoms of the independent unit. Two other peaks of medium height were considered spurious.

The coordinates were derived by the method of Shoemaker (1950). A structure factor calculation using a $B = 3{\cdot}5$, derived from Wilson statistics for all the atoms, gave a value of $R = 0{\cdot}31$ for the reliability index.

Two further cycles of structure factor calculation and three-dimensional Fourier synthesis lowered the value of R to $0{\cdot}19$. In this stage an isotropic temperature factor for each atom derived from the maximum value of each electron density peak of the Fourier synthesis was introduced (Damiani, Giglio & Ripamonti, 1963). The spurious peaks disappeared from the last three-dimensional Fourier synthesis that showed most of the details of the structure, the validity of which was studied by calculating all possible intra- and inter-molecular distances. Furthermore one oxygen atom had an electron density as low as 60% of the average of the other oxygen atoms. The possibility that this was due to a wrong position of this atom was considered and a Fourier synthesis was calculated with a set of structure factors computed without the contribution of this atom. This result confirms its position, and an attempt to weight down the contribution of this atom as due to a statistical vacancy increased the value of R. At this point it became clear that this effect was due to a large vibration of the particular oxygen atom in question.

The structure was refined by differential synthesis cycles and anisotropic temperature factors were introduced for each atom by comparison of the observed and calculated electron density curvatures. After several cycles the R index went down to $0{\cdot}12$, and at this point the positions of HMT hydrogen atoms were calculated and introduced into the structure factor calculations, with an isotropic temperature factor $B = 6{\cdot}0$ Å^2. The refinement was concluded when the coordinate shifts were of the order of one fourth of the estimated standard deviations, and the differences between the observed and calculated second derivatives of the electron density were less than 3%. The final value of the disagreement index is $R=0{\cdot}108$, including all the observed reflexions.

In Table 2 are listed the observed and calculated values of the structure factors based upon the final differential synthesis. In Table 3 are listed the atomic fractional coordinates and their standard deviations (Å) estimated according to Cruickshank (1949). The standard deviations of electron density and the first derivatives are $\sigma(\varrho)=0{\cdot}19$ e.Å^{-3}, $\sigma(A_h)=0{\cdot}51$ e.Å^{-4}, $\sigma(A_k)=0{\cdot}49$ e.Å^{-4}, $\sigma(A_l)=0{\cdot}48$ e.Å^{-4}. In Table 4 are listed the thermal parameters b_{11}, b_{12} *etc.* defined by the expression $\exp\left[-\left(b_{11}h^2+b_{12}hk+b_{13}hl+b_{22}k^2+b_{23}kl+b_{33}l^2\right)\right]$. The electron densities and their curvatures at the atomic positions are listed in Table 5.

Discussion

A diagrammatic representation of the structure can be seen in Fig. 1, where the hydrogen bonding system between the $Ca(H_2O)_6^{2+}$ octahedron, the HMT molecules, and the O(4) and O(5) water oxygen atoms which are not coordinated to the calcium ion is shown. The three crystallographically independent oxygen atoms of the water surrounding the calcium ion are hydrogen bonded to three nitrogen atoms of three different HMT molecules and to O(4), O(5) and Br respectively. Each group of atoms CaO(1)N(1)Br, CaO(2)N(3)O(5), CaO(3)O(4)N(4) is very nearly planar, and each plane is in a staggered position with respect to the other planes and makes an angle of about 20° with respect to an octahedral plane defined

Table 5. *Peak heights* (e.Å^{-3}) *and curvatures* (e.Å^{-5})

Values in parentheses are from F_c differential synthesis

	Peak height	$-A_{hh}$	A_{hk}	A_{hl}	$-A_{kk}$	A_{kl}	$-A_{ll}$
C(1)	7·68 (7·66)	57·4 (57·0)	28·6 (28·6)	7·8 (7·6)	65·0 (64·6)	9·6 (9·6)	59·2 (58·4)
C(2)	7·81 (8·06)	63·0 (64·0)	31·0 (30·8)	23·2 (22·8)	65·6 (66·0)	1·8 (1·4)	69·8 (70·4)
C(3)	8·19 (8·04)	62·8 (63·0)	35·8 (35·4)	9·2 (9·4)	71·4 (71·8)	9·8 (9·8)	68·0 (67·6)
C(4)	7·67 (7·79)	59·2 (60·6)	38·4 (37·6)	11·4 (11·4)	69·0 (68·6)	6·4 (6·0)	60·4 (60·4)
C(5)	8·19 (8·11)	66·4 (66·6)	35·4 (34·8)	17·8 (18·0)	61·8 (62·2)	−2·4 (−2·2)	75·0 (74·4)
C(6)	7·67 (7·61)	62·0 (61·4)	26·4 (26·6)	14·0 (14·2)	57·0 (56·4)	3·8 (3·8)	60·8 (60·4)
N(1)	9·93 (10·25)	93·2 (93·4)	41·0 (40·2)	19·2 (78·6)	78·8 (78·6)	11·4 (11·0)	86·8 (86·8)
N(2)	10·38 (10·14)	84·8 (85·0)	44·2 (44·0)	13·4 (13·4)	85·6 (85·4)	8·4 (8·2)	77·4 (77·4)
N(3)	9·61 (9·57)	71·2 (70·8)	37·2 (36·4)	11·0 (10·8)	74·4 (74·2)	6·2 (6·2)	80·6 (80·0)
N(4)	10·12 (10·23)	82·0 (81·8)	36·8 (37·0)	18·8 (19·0)	82·0 (81·8)	8·2 (8·2)	87·6 (87·6)
O(1)	10·02 (10·13)	87·0 (87·0)	41·2 (38·6)	18·8 (18·0)	73·8 (74·4)	13·4 (13·0)	65·4 (66·2)
O(2)	10·60 (10·54)	80·6 (79·8)	42·4 (43·0)	3·6 (3·6)	88·8 (88·4)	10·2 (11·2)	68·8 (68·6)
O(3)	10·65 (10·68)	91·2 (91·2)	34·8 (35·4)	19·0 (19·2)	78·6 (78·2)	0·4 (0·2)	75·6 (75·4)
O(4)	6·75 (6·35)	33·0 (35·0)	21·4 (20·8)	7·4 (9·6)	40·2 (42·0)	−7·0 (−1·6)	41·6 (41·6)
O(5)	10·56 (10·36)	76·8 (77·0)	35·4 (36·2)	4·2 (4·8)	74·2 (74·4)	0·6 (0·6)	82·8 (81·4)
Ca	43·52 (43·62)	431·8 (431·4)	21·4 (21·4)	74·4 (74·6)	420·4 (418·0)	41·0 (41·4)	400·6 (400·4)
Br	57·31 (57·38)	467·2 (463·6)	200·8 (201·2)	59·2 (58·8)	453·2 (452·8)	123·2 (121·8)	499·6 (496·6)

by the calcium ion and four oxygen atoms. In this way a second shell of atoms is formed around the Ca^{2+} that may resemble a distorted icosahedron (Fig. 2). The interatomic distances and bond lengths are given together with their estimated standard deviations in Table 6.

The deviations of the $Ca(H_2O)_6^{2+}$ octahedral angles from cubic symmetry are significant, whereas the Ca–O bond lengths are practically constant, an effect that is usually observed in such hydrate structures. The mean Ca–O distance of 2·34 Å is in agreement with the sum of the corresponding ionic radii.

The HMT parameters are all independent and their mean values are in good agreement with those found by Becka & Cruickshank (1963) in the crystal structure analysis of HMT. Although the variation of the parameters is very small, it is larger than the estimated standard deviations, and can be ascribed to crystal packing.

The bromine ion has three rather short contacts to O(1) (3·29 Å), O(4) (3·31 Å) and O(5) (3·30 Å), almost in a plane parallel to (001). Since the water oxygen atoms linked to the calcium ion have to be considered as proton donors to the nitrogen and oxygen atoms and to bromine ions of the second shell, it follows that O(5) and O(4) are proton donors to N(3) and Br^-, and to Br^- respectively. This hydrogen bond scheme is in agreement with bond angles [Table 6(*c*)].

Table 6. *Interatomic distances and bond angles*

The standard deviations are given in brackets.

(*a*) Coordination octahedron around Ca

Distances		Angles	
Ca–O(1)	2·316 (0·007) Å	O(1)–Ca–O(2)	93·3°(0·21°)
Ca–O(2)	2·330 (0·006)	O(1)–Ca–O(3)	84·3 (0·23)
Ca–O(3)	2·345 (0·006)	O(2)–Ca–O(3)	84·0 (0·22)
Mean value	2·330	O(1)–Ca–O(2′)	86·7 (0·21)
		O(1)–Ca–O(3′)	95·7 (0·23)
O(1)–O(2)	3·379 (0·009) Å	O(2)–Ca–O(3′)	96·0 (0·22)
O(1)–O(2′)	3·188 (0·009)		
O(1)–O(3)	3·126 (0·009)		
O(1)–O(3′)	3·456 (0·009)		
O(2)–O(3)	3·129 (0·009)		
O(2)–O(3′)	3·473 (0·009)		

(*b*) Hexamethylenetetramine molecule

Distances		Angles	
C(1)–N(1)	1·474 (0·010) Å	C(1)–N(1)–C(2)	109·0°(0·57°)
C(2)–N(1)	1·488 (0·009)	C(1)–N(1)–C(4)	107·1 (0·56)
C(4)–N(1)	1·477 (0·010)	C(2)–N(1)–C(4)	108·7 (0·56)
C(1)–N(2)	1·500 (0·010)	C(1)–N(2)–C(3)	107·5 (0·56)
C(3)–N(2)	1·473 (0·009)	C(1)–N(2)–C(5)	108·5 (0·57)
C(5)–N(2)	1·480 (0·009)	C(5)–N(2)–C(3)	109·7 (0·56)
C(2)–N(3)	1·473 (0·010)	C(2)–N(3)–C(6)	107·9 (0·59)
C(3)–N(3)	1·487 (0·010)	C(2)–N(3)–C(3)	106·7 (0·61)
C(6)–N(3)	1·459 (0·010)	C(3)–N(3)–C(6)	108·5 (0·60)
C(4)–N(4)	1·482 (0·010)	C(4)–N(4)–C(5)	107·5 (0·57)
C(5)–N(4)	1·474 (0·010)	C(4)–N(4)–C(6)	107·9 (0·57)
C(6)–N(4)	1·506 (0·010)	C(5)–N(4)–C(6)	108·1 (0·55)
		N(1)–C(1)–N(2)	110·7 (0·63)
		N(1)–C(2)–N(3)	112·7 (0·57)
		N(2)–C(3)–N(3)	112·5 (0·55)
		N(1)–C(4)–N(4)	112·6 (0·58)
		N(2)–C(5)–N(4)	111·2 (0·56)
		N(3)–C(6)–N(4)	113·0 (0·63)

	Present paper	Becka & Cruickshank (1963)
$(\text{C–N})_{av}$	1·481 Å	1·478 Å
$(\text{C–}\hat{\text{N}}\text{–C})_{av}$	108·1°	107·50°
$(\text{N–}\hat{\text{C}}\text{–N})_{av}$	112·1°	113·30°

(*c*) Hydrogen bonds

Distances		Angles	
O(1)–N(1)	2·829 (0·009) Å	Br—O(1)–N(1)	93·9°(0·22°)
O(1)–Br	3·291 (0·007)	O(5)–O(2)–N(2)	104·0 (0·28)
O(2)–N(2)	2·805 (0·008)	O(4)–O(3)–N(4)	101·8 (0·39)
O(2)–O(5)	2·743 (0·009)	Ca —O(1)–N(1)	127·7 (0·29)
O(3)–N(4)	2·831 (0·009)	Ca —O(1)–Br	138·3 (0·24)
O(3)–O(4)	2·711 (0·014)	Ca —O(2)–N(2)	128·4 (0·27)
O(5)–N(3)	2·868 (0·008)	Ca —O(2)–O(5)	127·5 (0·27)
O(5)–Br	3·298 (0·007)	Ca —O(3)–O(4)	129·1 (0·41)
O(4)–Br	3·312 (0·013)	Ca —O(3)–N(4)	126·6 (0·28)
		N(3)–O(5)–O(2)	121·6 (0·30)
		Br—O(5)–O(2)	103·9 (0·23)
		N(3)–O(5)–Br	94·6 (0·22)

(*d*) Ca–Br 5·250 (0·001) Å

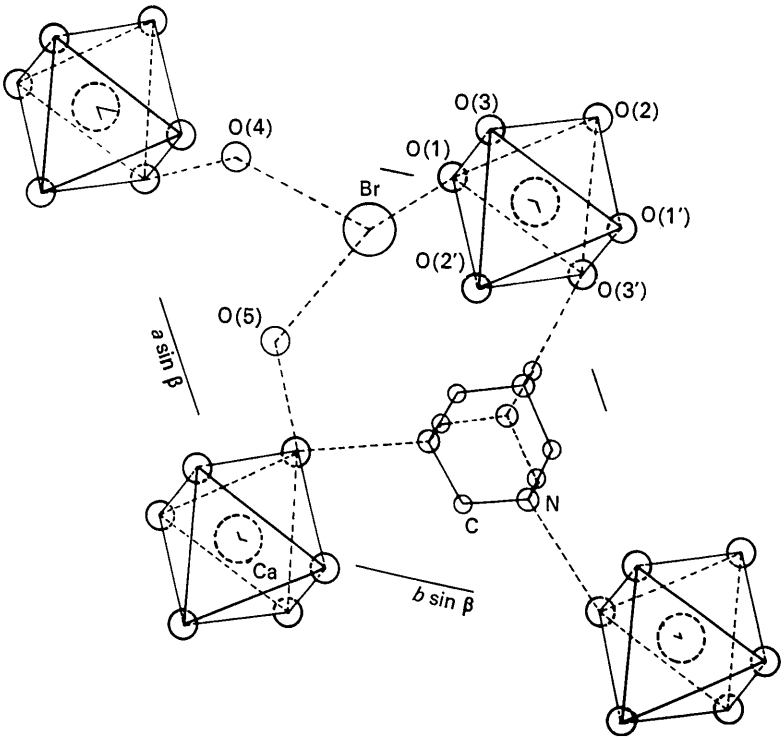

Fig. 3. View of the structure along the *c* axis.

The structure viewed along the *c* axis (Fig. 3) shows an approximately threefold symmetry. The HMT molecule projects at the centre of a triangle of $Ca(H_2O)_6^{2+}$ octahedra and connects them by hydrogen bonds. The bromine ion itself is almost at the centre of a triangle formed by three oxygen atoms, which lie in a plane approximately parallel to (001).

The structure can be considered as a layer structure parallel to the (001) plane. Within the layers electrostatic, van der Waals and hydrogen-bond forces stabilize the structure. The layers are held together by the longest hydrogen bonds present in the structure [O(5)–N(3)] and by weak van der Waals forces. These characteristics thus explain the perfect cleavage of the crystals along (001).

The triclinic crystals transform easily above room temperature in the presence of a small amount of water into the cubic modification (which has a much lower solubility). If there is sufficient water a macroscopic dissolution process is visible and a subsequent crystallization gives cubic crystals. If the crystals are just wet, then they keep the triclinic shape but loose the birefringence and show a disordered X-ray diffraction pattern. Probably a microdissolution process takes place, and the fact that the process can occur at all has to be related to a close similarity between the two forms. Indeed if a (001) layer of the triclinic structure is shifted along the [110] direction so to bring a Ca^{2+} ion to the centre of a triangle between calcium ions of an upper level, the structure obtained is very close to that of the cubic form. Thus epitaxic growth of the cubic form on the triclinic form can be explained in these terms. The orientation of the cubic reciprocal lattice with respect to the triclinic reciprocal axis can be calculated and compared with that found experimentally on an X-ray diffraction photograph of a crystal containing both forms. The orientation of the reciprocal lattices agrees perfectly with what we expected.

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