Inorganica Chimica Acta, 13 (1975) 149–161
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The Crystal and Molecular Structure of Pentakis(diacetamide)barium(II) Perchlorate

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Received September 19, 1974

The crystal structure of pentakis(diacetamide)barium(II) perchlorate, $[Ba((CH_3CO)_2NH)_5](ClO_4)_2$, has been determined from three-dimentional X-ray diffraction data using CuKα radiation. The unit cell constants are a = 13.052(5)A, b = 14.406(6) Å, c = 19.508(8) Å and β = 107.6(3)°. The monoclinic colorless crystals belong to the space group $P2_1/c$. The observed and calculated (Z = 4) densities are 1.608 g/cm³ and 1.602 g/cm³ respectively. Two sets of intensity data (nkl and hnl) were recorded on film by the equi-inclination Weissenberg method and their intensities estimated visually. A total of 4041 independent reflections above background were used in the Patterson and Fourier summations for structure determination. The structure was refined by full-matrix least squares to an unweighted conventional R factor of 0.094. The five diacetamide molecules assume a modified trans–trans (diacetamide-B) configuration with a small twist from planarity (5–15°) about the oxygen–oxygen line as they bond as bidentates to barium forming a ten co-ordinated complex. The six membered rings formed by the diacetamide ligand with barium are folded to varying degrees (7–42°) about the oxygen–oxygen lines. The bonded oxygen atoms are located at the vertexes of a distorted symmetrically bicapped square antiprism (D_{4d}). Barium–oxygen bond distances vary from 2.73(2) Å to 2.91(2) Å. The complex is unique in that it is the first reported case of a ten co-ordinated complex, characterized by X-rays, where all of the ligands are non-ionic, chemically identical bidentates. The hybrid orbitals of barium that could reasonably be involved in sigma covalent bonding with the oxygen atoms are $sp^3d^5f_{z(5z^2-3r^2)}$.

Introduction

Reactions of diacetamide (DA) with alkaline earth salts were reported to yield complexes of unusual co-ordination[1,2]. Two of the compounds, $[Ca(DA)_5](ClO_4)_2$ and $[Ba(DA)_5](ClO_4)_2$, were postulated as having a co-ordination number of nine[1,2]. Such a high co-ordination number for alkaline earth complexes is unusual[3] but reasonable. Since the structure of only few nine co-ordinate complexes has been reported[4–9] a single crystal X-ray structural determination of pentakis(diacetamide)barium(II) perchlorate was undertaken in order to establish unequivocally the structure of the compound and to help explain infrared data previously obtained.

Experimental

Preparation

Diacetamide, prepared by the acylation of acetamide with acetic anhydride[10], was recrystallized from ethyl ether. Anhydrous barium perchlorate and diacetamide in the molar ratio of 1:12 were mixed and 5 ml increments of dry acetone were added to dissolve the mixture. Large crystals of the barium complex obtained by slow addition of ethyl ether to the acetone solution were collected and washed with portions of ethyl ether to remove excess diacetamide. The infrared spectrum was identical to that reported[1,2]. *Anal.* Calcd. for $Ba(DA)_5(ClO_4)_2$: Ba, 16.32. Found Ba, 16.87%.

X-Ray

The density of the crystals were determined by the flotation method using methyl iodide and carbon tetrachloride. Three crystal were mounted perpendicular to one another and each inserted inside sealed quartz capilaries. Lattice parameters were determined at room temperature using nickel-filtered copper radiation. Unit cell translations were evaluated from rotation photographs by extrapolation to a Bragg angle of 90°. The error is the standard deviation of the intercept. The monoclinic angle, β, was measured from a Weissenberg photograph of the h0l zone. The error reported is the standard deviation of the mean. Oscillation and preliminary Weissenberg photographs (0kl, 1kl, h0l, h1l) indicated that the crystals belong to the space group $P2_1/c$ within the monoclinic system. Four molecules of $Ba(DA)_5(ClO_4)_2$ are present per unit cell. The crystal data are listed in Table I.

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TABLE I. Crystallographic Data for $[Ba((CH_3CO)_2NH)_5](ClO_4)_2$.

M.W. = 841.77
Crystallographic system: monoclinic
Space group: $P2_1/c$
Unit cell parameters: $a = 13.052(5)A^a$
$b = 14.406(6)A$
$c = 19.503(8)A$
$\beta = 107.6(3)°$
$V = 3490.9A^3$
$Z = 4$
$d_{calcd} = 1.602\ g/cm^3$ $\mu_{CuK\alpha} = 103.1\ cm^{-1}$
$d_{obs} = 1.608\ g/cm^3$ $\lambda = 1.5418A$
$F_{000} = 1584$

[a] The quantities enclosed in brackets are the estimated standard deviations.

Two sets of intensity data were collected by the multiple-film equi-inclination Weissenberg technique: one set (h0l–h10l) using a crystal mounted about the *b*-axis and of dimensions 0.08, 0.5, 0.1 mm (*a,b,c*), and another set (0kl–10kl) using a crystal mounted about the *a*-axis and of dimensions 0.11, 0.23, 0.23, 0.13 mm (*a,b,c,n*) and bound by the faces (100), (010), (101). The intensities were estimated visually by means of comparison with calibrated strip made by timed exposure of a selected reflection in a Weissenberg film of the corresponding crystal. Correction for spot shape differences were also estimated visually. A total of 3650 independent reflections out of 6461 possible ones in the nkl set, and a total of 2351 out of 6009 in the set hnl, were observable. The raw intensities were corrected for Lorentz and polarization effects[11]. Cylindrical absorption corrections were applied to the data from the *b*-mounted crystal[12]. The absorption term for the *a*-mounted crystal, however, is more complex because of the shape and morphology. The problem was by-passed by using the same μR value for all the nkl layers, where R is the radius for each of the layers 0kl–10kl. Doing this, absorption correction as a function of $\sin\Theta$ were made within each layer, but variation in cylindrical absorption factors between layers due to changes in R were not taken into consideration. The layer absorption factor was incorporated in the layer scaling factor upon intercorrelation of data from two axes. Reflections within each of the sets nkl and hnl were intercorrelated with data from the other set thus putting them all on a common scale. A total of 4041 non-zero independent reflections, obtained after combining the two sets, were used for structure determination.

Solution and refinement

The phases of the structure factors are dominated by contributions from the barium atoms as the ratio $Z^2_{heavy}/\Sigma Z^2_{light}$ is 1.15. The abundance of intensity data from two axes rendered the parameters of the light atoms more defineable. A three-dimensional Patterson summation[13] revealed the co-ordinates of the barium atom. A three-dimensional Fourier summation[14] phased on the barium atom alone was sufficient to reveal the approximate positions of the remaining fourty-five atoms in the asymmetric unit. Very few minor peaks were observed. The R factor at this point was 0.34. The inclusion in the Fourier summation of the fourty-five non-hydrogen atoms reduced the R factor to 0.22 and the intensity of the superfluous peaks to negligible values.

A least squares diagonal matrix approximation[15] was used for the initial refinement of the structure and reduced the isotropic unweighted R factor to 0.131. Subsequent full matrix least squares refinement[16], using a CDC6600 computer, reduced the isotropic unweighted R factor to 0.128. A difference electron density array run at this point showed some anisotropy in the thermal vibration of the barium atom, and except in the vicinity of the barium atom, the residual peaks had an intensity of less than 0.7 e/A^3. Exclusion from refinement of 73 reflections with intensities at the limit of observability[17] brought the unweighted isotropic R factor to 0.123 and the weighted isotropic R factor to 0.138. A variance-covariance matrix was also obtained at the end of this cycle and was later used in the evaluation of standard deviations in bond lengths and angles[18]. Calculation and assignment of anisotropic temperature factors for all of the atoms resulted in a final unweighted R factor of 0.094 and a final weighted R factor of 0.113. The maximum shift in the last cycle of refinement was less than 0.01σ.

The mean atomic scattering factors for neutral barium were those calculated by L. H. Thomas and K. Umeda from the Thomas–Fermi–Dirac statistical model[19] and were corrected for real and imaginary dispersion effects[20]. The function minimized in the least squares fit is $\Sigma w(|F_0|-k|F_c|)^2$ where w is a weighting factor. The unweighted R factor, R, is defined as $\Sigma(|F_o|-k|F_c|)/\Sigma|F_o|$, and the weighted R factor, wR, as $[\Sigma w(|F_o|-k|F_c|)^2/\Sigma w|F_o|^2]^{1/2}$. The scale factor, k, was treated as an additional parameter. Empirical weighting schemes were attempted but all gave worse values of R and wR than weighting all observations equally. The latter procedure was therefore adopted. The unobserved planes were not included in the calculation of the residual, and no reflections were excluded from refinement due to extinction effects.

Table II gives the observed and calculated structure amplitude, $|F_o|$ and $|F_c|$. The fractional co-ordinates and the isotropic thermal parameters of all atoms are listed in Table III. The atom designation for the DA ligands are according to Figure 1. The anisotropic thermal parameters are listed as mean square amplitude, U_{ij}, in Table IV. All bond distances are listed in Table V with other relevent interatomic distances between non-bonded or hydrogen bonded atoms listed

TABLE II. Observed and Calculated Structure Amplitude ($F_{000} = 1584$).

K = 0

H	L	FOBS	FCALC
0	2	36	37
0	4	41	39
0	6	116	198
0	8	194	199
0	10	79	91
0	12	88	79
0	16	109	109
0	20	32	30
1	2	132	150
1	4	156	143
1	6	92	87
1	8	141	143
1	10	100	96
1	12	91	87
1	14	74	75
1	16	42	42
1	20	35	45
1	-2	149	161
1	-4	156	172
1	-6	271	279
1	-8	202	202
1	-12	100	96
1	-14	71	72
1	-16	91	99
1	-20	41	39
2	0	136	173
2	2	112	117
2	4	112	108
2	6	209	211
2	8	90	92
2	10	119	111
2	12	39	31
2	14	56	48
2	16	59	53
2	18	52	49
2	20	29	24
2	22	30	33
2	-2	133	159
2	-4	55	58
2	-6	117	119
2	-8	133	133
2	-10	159	177
2	-12	69	71
2	-14	47	40
2	-16	50	50
2	-18	39	43
2	-20	24	23
2	-22	33	35
3	0	92	103
3	2	220	256
3	4	34	24
3	6	209	213
3	8	19	13
3	10	114	111
3	12	61	60
3	14	77	79
3	16	17	21
3	18	40	43
3	-2	69	68
3	-4	233	250
3	-6	132	135
3	-8	109	112
3	-10	116	116
3	-14	126	135
3	-16	25	22
3	-18	39	43
3	-20	19	23
3	-22	17	24
4	2	26	28
4	4	50	42
4	6	167	181
4	8	22	17
4	10	119	120
4	12	59	63
4	14	59	60
4	16	38	36
4	18	25	24
4	20	24	21
4	-2	254	285
4	-4	97	97
4	-6	190	200
4	-8	43	32
4	-10	122	116
4	-12	23	17
4	-16	95	95
4	-18	65	70
4	-22	31	36
5	0	31	40
5	2	224	239
5	4	95	95
5	6	50	51
5	8	64	69
5	10	66	60
5	12	57	58
5	14	41	40
5	16	33	31
5	18	17	21
5	20	21	28
5	-2	60	78
5	-4	119	121
5	-6	152	161
5	-8	108	117
5	-10	129	137
5	-14	99	93
5	-16	30	32
5	-18	43	47
5	-20	14	33
5	-22	35	36
6	0	106	107
6	2	93	102
6	4	105	109
6	6	56	55
6	8	45	37
6	12	66	63
6	14	29	30
6	16	45	46
6	-2	104	132
6	-4	122	141
6	-6	59	62
6	-8	106	103
6	-10	61	55
6	-12	115	117
6	-14	79	79
6	-16	34	35
6	-18	42	42
6	-20	29	29
7	0	162	191
7	2	17	16
7	4	32	32
7	6	17	17
7	8	113	117
7	12	76	76
7	16	37	34
7	-2	72	77
7	-4	117	114
7	-6	106	110
7	-8	116	113
7	-10	55	44
7	-12	47	42
7	-16	45	49
7	-20	32	33
8	0	37	36
8	2	53	58
8	4	139	145
8	6	17	17
8	8	45	41
8	10	54	55
8	12	54	55
8	16	29	31
8	-2	56	61
8	-4	163	167
8	-6	59	54
8	-8	41	75
8	-10	22	23
8	-12	93	91
8	-14	36	41
8	-16	35	31
8	-18	22	23
8	-20	36	40
8	-24	17	28
9	0	101	106
9	2	54	60
9	4	36	36
9	6	126	132
9	8	41	38
9	10	45	44
9	12	24	26
9	14	42	52
9	-2	70	74
9	-4	16	16
9	-6	27	26
9	-8	59	61
9	-10	44	57
9	-12	54	47
9	-14	21	9
9	-16	62	63
9	-18	29	26
9	-20	24	26
10	2	96	96
10	6	46	47
10	10	59	62
10	14	60	63
10	-2	104	126
10	-4	64	70
10	-6	81	83
10	-10	41	37
10	-12	23	21
10	-14	56	56
10	-16	22	21
10	-18	51	46
10	-20	28	29
11	2	45	44
11	2	45	44
11	4	31	35
11	6	51	60
11	-2	73	75
11	-6	88	89
11	-10	74	68
11	-14	49	46
12	0	44	44
12	2	75	83
12	6	27	33
12	8	63	51
12	-6	55	53
12	-8	74	64
12	-14	66	58
12	-16	29	4
13	0	65	73
13	4	49	54
13	8	35	45
13	-6	44	41
13	-10	43	45
13	-12	42	40
14	0	45	53
14	4	35	43
14	-8	69	69
15	0	29	32
15	-12	32	31

K = 1

H	L	FOBS	FCALC
0	2	223	253
0	4	132	136
0	5	93	76
0	6	178	187
0	7	85	85
0	8	40	40
0	9	33	34
0	10	178	173
0	11	34	36
0	12	40	35
0	13	51	49
0	14	46	42
0	16	25	23
0	18	56	60
0	22	25	32
1	0	26	31
1	1	21	26
1	2	180	220
1	3	64	67
1	4	296	340
1	5	35	37
1	6	106	114
1	7	83	79
1	8	86	87
1	9	27	21
1	10	67	68
1	12	37	39
1	13	28	8
1	14	101	104
1	16	32	26
1	18	46	48
1	20	37	40
1	22	20	23
1	-1	32	40
1	-2	210	280
1	-3	42	44
1	-4	70	64
1	-6	32	30
1	-7	23	18
1	-8	101	93
1	-10	102	89
1	-11	23	19
1	-12	46	44
1	-14	95	94
1	-16	33	25
1	-17	19	15
1	-19	38	41
1	-22	29	30
2	0	57	70
2	1	26	15
2	2	75	65
2	3	63	57
2	4	152	177
2	5	36	26
2	6	105	113
2	7	54	51
2	8	78	73
*2	9	23	1
2	10	70	71
2	11	23	19
2	12	90	93
2	13	35	31
2	16	57	55
2	18	33	30
2	20	39	34
*2	-1	11	1
2	-2	125	149
2	-3	95	98
2	-4	59	66
2	-5	211	211
2	-6	128	136
2	-7	137	141
2	-8	53	56
2	-9	32	26
2	-10	90	93
2	-11	30	29
2	-12	80	80
2	-13	29	23
2	-14	37	32
2	-15	51	49
2	-16	61	58
*2	-17	26	12
2	-18	71	74
3	0	27	31
3	1	15	9
3	2	119	127
3	3	44	46
3	4	183	188
3	5	53	46
3	8	185	193
3	9	17	5
3	11	19	16
3	12	106	112
3	16	35	36
3	20	39	39
*3	22	9	3
3	-1	56	49
3	-2	154	154
3	-4	214	239
3	-5	70	64
3	-6	136	141
3	-7	52	49
3	-8	193	197
3	-9	17	13
3	-10	46	51
3	-11	43	49
3	-12	54	54
3	-13	50	53
3	-14	45	45
3	-16	69	73
3	-17	31	13
3	-19	27	24
3	-20	23	22
3	-22	19	17
3	-24	16	26
4	0	185	234
4	1	68	65
4	2	53	56
4	3	46	49
4	4	171	173
4	5	37	34
4	6	74	71
4	8	69	60
4	10	33	29
4	12	49	45
4	13	34	32
4	14	29	22
4	16	67	69
4	18	16	16
4	20	29	27
4	-1	67	73
4	-3	16	22
4	-4	140	162
4	-5	60	46
4	-6	63	57
4	-7	52	51
4	-8	81	99
4	-9	36	33
4	-10	53	51
4	-11	25	30
4	-12	130	137
4	-15	22	22
4	-16	50	51
4	-20	43	47
*4	-23	26	3
4	-24	22	25
5	0	109	117
5	1	56	61
5	2	95	103
5	4	71	69
5	5	18	20
5	6	19	17
5	8	55	55
5	10	56	51
5	11	28	26
5	12	68	75
5	14	55	60
5	18	28	37
*5	19	20	2
5	20	19	21
5	-1	66	72
5	-4	82	92
*5	-5	20	5
5	-6	90	97
5	-7	18	18
5	-8	109	116
5	-9	19	18
5	-10	91	93
5	-11	27	23
5	-12	49	51
5	-14	25	20
5	-16	90	100
5	-18	21	23
5	-20	24	33
5	-24	17	19
6	0	67	79
6	1	38	37
6	2	85	91
6	3	28	29
6	4	88	86
6	5	14	9
6	6	68	76
6	8	58	59
6	10	98	94
6	14	70	74
6	18	29	33
6	-2	130	158
6	-4	63	63
6	-5	20	20
6	-6	114	120
6	-7	22	18
6	-8	114	119
6	-9	22	10
6	-10	68	66
6	-12	39	40
6	-14	41	38
6	-16	26	23
6	-18	44	43
6	-20	28	25
6	-22	27	32
7	0	12	8
7	1	27	32
7	2	153	162
7	3	14	11
*7	5	41	21
7	6	127	132
7	8	23	26
7	10	80	83
7	11	27	29
7	13	23	27
7	14	41	39
7	18	34	37
7	-2	92	110
7	-6	110	114
7	-7	34	25
7	-8	84	83
*7	-9	16	6
7	-10	149	150
7	-13	41	42
7	-14	64	67
7	-16	29	27
7	-18	41	47
7	-22	21	26
8	0	82	87
8	2	96	62
8	4	70	69
8	6	100	100
8	8	42	44
8	10	52	53
8	14	47	45
8	16	29	24
8	-1	13	16
8	-2	135	151
8	-3	17	19
8	-4	45	45
8	-6	80	78
8	-7	32	24
8	-8	32	30
8	-9	36	34
8	-10	56	55
8	-11	37	37
8	-12	50	50
8	-14	90	95
8	-18	31	29
8	-22	20	27
9	0	106	109
9	2	24	25
9	4	56	63
9	6	60	56
9	8	61	62
9	9	20	17
9	10	43	39
9	12	57	55
9	13	21	18
9	14	16	17
9	-2	52	58
*9	-3	12	3
9	-4	72	85
9	-6	71	72
9	-7	26	19
9	-8	35	33
9	-10	69	63
9	-11	16	10
9	-12	37	34
9	-16	38	32
9	-18	38	41
9	-20	28	26
9	-22	27	30
10	0	48	49
10	2	53	50
10	4	80	80
10	8	54	50
10	12	30	52
10	-2	33	33
10	-4	76	95
10	-5	19	24
10	-6	11	10
10	-8	94	91
10	-9	16	15
10	-10	33	26
10	-11	35	36
10	-12	66	65
10	-14	41	34
10	-16	32	33
10	-20	26	25
11	0	77	73
11	2	43	39
11	4	74	81
*11	7	37	14
11	8	29	40
11	12	36	42
11	-2	30	34
11	-4	96	97
11	-9	30	37
11	-12	78	84
12	0	40	45
12	2	60	55
12	4	49	54
12	8	33	45
12	10	36	40
12	-2	41	47
12	-6	49	50
12	-8	57	66
*12	-9	30	11
12	-16	30	39
13	0	28	33
13	2	45	52
13	4	25	25
13	5	23	2
13	6	51	51
13	8	24	29
13	-2	46	53
13	-6	47	49
13	-8	44	67
13	-10	29	43
13	-12	45	50
13	-18	21	19
14	2	49	57
14	6	32	35
14	-2	51	56
14	-6	51	53
14	-10	54	52
14	-14	33	39
14	-18	16	26
15	0	20	17
*15	1	18	13
15	2	34	29
15	-2	33	42
15	-6	47	47
15	-8	23	17
*15	-12	21	11
16	-4	24	26
16	-6	24	28
16	-8	18	19

K = 2

H	L	FOBS	FCALC
0	0	356	405
0	2	211	203
0	3	80	74
0	4	182	175
0	5	180	160
0	6	28	21
0	8	121	114
0	9	38	35
0	10	28	20
0	11	59	57
0	12	90	83
0	13	20	30
0	16	71	68
0	18	25	26
0	20	29	36
1	0	85	101
1	1	83	82
1	2	89	81
1	3	96	101
1	4	28	26
*1	5	19	9
1	7	34	34
1	6	122	119
1	8	158	167
1	9	92	93
1	10	50	44
1	11	55	51
1	12	58	60
1	13	37	38
1	14	78	80
1	16	27	23
1	20	35	35
1	-1	193	218
1	-2	123	137
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TABLE II. (Cont.)

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K = 6

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2	-13	49	51
2	-15	24	15
2	-17	36	38
3	1	88	90
3	3	108	97
3	5	53	49
3	6	31	30
3	7	31	35
3	8	31	24
3	9	30	32
3	10	25	24
3	11	45	44
3	15	33	37
3	17	23	30
3	-1	114	122
3	-2	44	43
3	-3	20	15
3	-4	23	20
3	-5	125	94
3	-7	37	38
3	-9	49	52
3	-11	43	57
3	-13	57	57
3	-17	45	47
4	0	26	20
4	1	74	68
• 4	2	27	8
4	3	24	29
4	4	19	16
4	5	80	77
4	7	69	60
4	9	61	59
4	11	37	37
4	13	46	49
4	17	25	25
4	-1	63	58
• 4	-2	18	5
4	-3	113	109
4	-4	37	42
4	-5	34	26
4	-6	40	47
4	-7	63	73
4	-9	67	74
4	-11	54	45
4	-15	34	39
4	-19	22	27
5	1	91	92
5	3	25	26
5	5	91	90
5	9	76	70
5	13	36	38

TABLE II. (Cont.)

K = 10

H	L	FOBS	FCALC
5	-2	24	20
5	-3	47	49
5	-5	24	26
5	-6	22	21
5	-7	100	103
5	-10	47	48
5	-11	37	37
5	-13	27	28
5	-15	23	31
5	-19	23	32
6	1	106	104
6	3	63	64
6	5	48	56
6	7	39	32
6	9	46	43
6	11	36	37
6	13	43	40
6	15	21	21
6	-3	73	78
6	-7	40	37
6	-9	32	38
6	-11	75	77
6	-15	44	46
6	-19	18	28
7	1	59	48
7	3	26	28
7	7	33	28
7	9	51	49
7	10	47	9
7	11	36	41
7	-1	88	91
7	-2	22	15
7	-3	43	40
7	-4	20	16
7	-5	32	30
7	-7	72	76
7	-9	46	48
7	-11	30	36
7	-13	23	20
7	-15	28	29
7	-17	24	24
7	-19	21	29
8	0	32	35
8	1	26	17
8	3	77	71
8	7	54	52
8	11	38	41
8	-1	24	23
8	-2	26	22
8	-5	75	66
8	-8	42	40
8	-9	50	56
8	-11	29	32
8	-13	32	34
8	-17	21	26
9	1	35	7
9	2	27	27
9	3	67	61
9	7	53	55
9	11	33	29
9	-1	63	59
9	-5	54	38
9	-9	57	63
9	-13	42	47
9	-17	18	21
10	1	44	45
10	3	53	51
10	7	32	31
10	9	23	20
10	-1	43	41
10	-3	22	19
10	-5	61	67
10	-9	43	39
10	-13	36	43
10	-17	19	22
11	5	38	41
11	-3	76	63
11	-5	36	22
11	-9	40	36
12	1	49	56
12	-7	40	49
13	3	25	31
13	-3	33	35

K = 11

H	L	FOBS	FCALC
0	1	30	17
0	2	24	32
0	3	100	95
0	5	53	49
0	7	74	70
0	9	97	108
0	11	55	61
0	13	40	40
0	17	17	19
0	18	14	3
0	19	14	16
1	0	32	30
1	1	118	105
1	2	26	20
1	3	27	27
1	5	116	104
1	7	27	29
1	9	45	50
1	13	42	48
1	17	29	35
1	-2	26	20
1	-3	76	69
1	-5	69	67
1	-7	79	62
1	-11	63	61
1	-13	36	43
1	-15	43	45
2	1	130	132
2	5	56	49
2	9	79	74
2	13	49	43
2	15	23	28
2	17	37	36
2	-1	35	38
2	-3	139	131
2	-5	46	52
2	-7	61	49
2	-11	67	72
2	-15	49	58
2	-17	19	7
2	-19	23	39
3	1	95	88
3	2	71	28
3	5	98	93
3	9	44	49
3	11	33	41
3	13	35	35
3	15	37	24
3	-1	95	87
3	-3	81	69
3	-5	63	63
3	-6	30	41
3	-7	121	124
3	-9	53	54
3	-11	56	59
3	-15	57	63
3	-17	22	26
3	-19	15	20
4	1	84	94
4	3	74	64
4	7	102	96
4	11	27	29
4	13	23	25
4	15	32	30
4	-1	61	57
4	-3	66	63
4	-5	79	69
4	-9	92	93
4	-11	68	69
4	-13	92	94
5	3	81	77
5	7	53	58
5	11	42	65
5	15	29	33
5	-1	92	97
5	-3	43	40
5	-5	72	76
5	-6	29	36
5	-9	49	43
5	-13	41	51
5	-17	39	45
5	-19	12	7
6	1	22	22
6	3	40	30
6	7	80	69
6	11	45	45
6	13	28	28
6	-1	78	75
6	-3	32	37
6	-5	83	80
6	-9	62	70
6	-13	42	45
6	-17	24	35
7	1	24	24
7	3	58	55
7	5	63	53
7	7	22	23
7	9	50	48
7	11	16	17
7	-1	74	73
7	-3	39	33
7	-7	42	47
7	-9	49	53
7	-11	35	36
7	-13	33	35
7	-17	29	44
8	0	23	27
8	1	64	41
8	5	57	53
8	9	24	32
8	-1	37	33
8	-3	58	53
8	-5	31	37
8	-7	53	54
8	-11	33	33
8	-15	36	38
8	-17	17	23
9	1	90	44
9	5	41	46
9	9	51	46
9	-3	57	53
9	-7	64	64
9	-11	41	40
9	-15	18	19
10	1	50	43
10	3	24	25
10	5	40	45
10	7	29	29
10	-1	22	23
10	-3	22	25
10	-5	19	16
10	-7	56	56
10	-9	21	26
10	-11	42	48
10	-15	25	29
10	-17	9	16

K = 12

H	L	FOBS	FCALC
0	0	37	44
0	1	68	64
0	2	90	93
0	3	71	69
0	4	31	29
0	5	36	34
0	6	31	31
0	7	67	72
0	9	44	46
0	11	30	33
0	13	31	33
0	17	14	20
1	0	27	27
1	3	71	56
1	5	47	46
1	6	34	26
1	7	79	80
1	11	38	65
1	15	36	44
1	-1	73	67
1	-2	33	34
1	-5	118	113
1	-7	34	36
1	-8	27	34
1	-9	45	40
1	-10	19	18
1	-11	29	31
1	-13	41	38
1	-15	14	16
1	-17	31	36
2	0	64	53
2	2	26	20
2	3	78	70
2	4	43	50
2	7	75	64
2	11	46	40
2	13	20	10
2	15	44	47
2	-1	90	91
2	-2	37	32
2	-4	32	28
2	-5	80	75
2	-9	81	82
2	-13	47	41
*2	-15	20	9
2	-17	27	34
3	1	56	48
3	3	86	81
3	4	29	26
3	5	54	53
3	7	30	29
3	9	29	29
3	11	37	33
3	13	28	32
3	15	30	32
3	-1	121	123
3	-3	25	21
3	-5	53	47
3	-7	36	36
3	-9	51	47
3	-11	37	38
3	-13	46	45
3	-17	27	34
4	1	57	46
4	3	65	61
4	7	90	52
4	9	50	48
4	13	45	46
4	-1	37	33
4	-3	102	107
4	-5	44	42
4	-6	23	24
4	-7	36	38
4	-9	55	56
4	-11	46	53
4	-15	27	22
5	0	39	36
5	1	59	59
5	5	73	80
5	9	54	58
5	13	28	31
5	-3	56	58
5	-7	64	63
5	-9	22	20
5	-11	47	59
5	-15	27	28
6	1	82	77
6	3	39	44
6	5	74	71
6	7	23	21
6	9	35	43
6	13	32	36
6	-3	64	65
6	-6	26	31
6	-7	37	34
6	-11	52	54
6	-15	34	45
7	1	42	42
7	3	39	41
7	5	34	35
7	7	26	30
7	9	32	26
7	11	28	34
7	-1	54	51
7	-3	70	64
7	-4	34	26
7	-5	49	54
7	-7	42	43
7	-9	26	29
7	-11	28	34
7	-13	20	24
7	-15	20	34
8	3	65	53
8	7	30	38
8	-3	26	28
8	-5	72	73
8	-1	37	37
8	-9	46	44
8	-11	28	25
8	-13	25	34
8	-17	15	20
9	3	46	50
9	7	37	34
9	-1	53	48
9	-5	41	43
9	-9	43	43
9	-13	34	41
9	-17	15	22
10	1	25	27
10	3	35	38
10	5	17	19
10	-1	40	38
10	-3	20	25
10	-5	40	41
10	-9	34	47
10	-13	28	33
10	-15	10	13

K = 13

H	L	FOBS	FCALC
0	1	31	25
0	2	48	60
0	3	69	63
0	4	25	21
0	5	70	77
0	7	55	54
0	9	56	47
0	13	34	41
0	14	17	20
0	15	15	23
1	1	64	63
1	5	72	70
1	8	26	33
1	9	40	35
1	13	33	45
1	-3	76	78
1	-4	33	33
1	-5	27	15
1	-7	46	49
1	-11	50	49
1	-13	26	32
1	-15	17	23
1	-17	16	18
2	1	72	57
2	5	55	59
2	9	46	41
2	13	50	53
2	15	13	16
2	-3	66	55
2	-7	53	57
2	-9	25	25
2	-11	23	27
2	-15	34	46
3	1	61	61
3	2	25	28
3	5	42	43
3	7	38	46
3	8	26	22
3	9	48	48
3	11	37	36
3	13	22	21
3	15	19	27
3	-1	50	51
3	-3	56	55
3	-5	39	28
3	-7	52	53
3	-11	40	55
4	0	23	17
4	1	23	31
4	5	77	78
4	7	54	49
4	11	38	39
4	13	16	17
4	-1	46	49
4	-3	37	37
4	-5	34	38
4	-7	33	36
4	-9	45	46
4	-11	32	32
4	-15	23	23
5	3	59	58
5	7	51	59
5	11	35	43
5	-1	52	57
5	-5	53	60
5	-9	37	49
5	-13	46	48
*5	-19	17	3
6	1	28	25
6	3	56	59
6	7	62	67
6	9	18	22
6	11	27	28
6	-1	47	47
6	-3	25	22
6	-5	62	51
6	-8	27	19
6	-9	52	62
6	-13	20	24
6	-17	16	28
7	1	35	42
7	3	43	36
7	5	36	44
7	7	30	34
7	9	20	21
7	-1	49	60
7	-2	19	26
7	-3	31	33
7	-5	25	29
7	-7	38	41
7	-9	37	43
7	-13	19	24
7	-17	8	17
8	1	61	58
8	9	43	45
8	-1	23	25
8	-3	49	53
8	-7	43	47
8	-11	29	42
9	1	50	47
9	5	36	43
9	-3	40	44
9	-7	41	42
9	-11	26	33
9	-15	19	25
10	1	37	42
10	3	23	23
10	-1	16	20
10	-3	23	31
10	-5	19	19
10	-7	30	31
10	-11	29	40

K = 14

H	L	FOBS	FCALC
0	0	47	35
0	1	49	53
0	3	69	63
0	5	24	21
0	7	44	44
0	9	25	26
0	11	33	32
0	13	29	35
0	15	22	26
1	0	33	43
1	2	26	23
1	3	37	39
1	7	73	77
1	11	32	39
1	15	21	32
1	-1	84	75
*1	-4	26	9
1	-5	41	31
1	-7	31	32
1	-9	49	55
1	-13	29	29
1	-15	13	15
2	0	25	23
2	3	82	84
2	6	36	32
2	7	49	45
2	9	30	32
2	11	39	38
2	-1	36	36
2	-3	50	48
2	-6	24	11
2	-7	29	30
2	-9	45	52
2	-13	25	34
3	1	29	32
3	3	42	41
3	5	41	41
3	7	30	29
3	10	23	30
3	11	28	25
3	13	20	28
3	-1	82	84
3	-2	37	33
3	-3	32	37
3	-9	39	32
3	-10	21	24
3	-11	17	31
*3	-12	19	7
3	-13	27	29
*3	-15	13	5
4	1	49	42
4	3	31	23
4	5	30	31
4	6	23	28
4	9	48	45
4	10	22	29
4	-1	22	21
4	-2	37	33
4	-3	45	56
4	-5	43	48
4	-7	40	35
4	-11	27	28
4	-13	19	27
4	-15	18	20
5	1	30	28
5	5	46	53
5	6	20	17
5	9	37	54
5	-5	57	57
5	-7	40	45
5	-11	33	48
5	-15	27	29
6	0	23	27
6	1	67	66
6	5	33	36
6	7	25	28
6	9	35	40
6	-3	37	36
6	-7	40	49
6	-11	35	29
*6	-15	21	40
7	0	28	29
7	1	28	27
7	3	33	34
7	4	18	18
7	5	30	38
7	7	20	20
7	8	13	18
7	-1	34	38
7	-3	48	51
7	-4	18	16
7	-5	39	46
7	-7	28	35
7	-11	21	25
7	-13	16	25
7	-15	16	26
8	0	17	24
8	3	33	32
8	-1	41	37
8	-5	36	44
8	-9	39	39
8	-13	15	16
9	2	13	17
9	3	53	54
9	-1	29	30
9	-5	36	40
9	-9	30	34
9	-13	18	17
10	1	12	19
10	-3	21	22
10	-5	22	26
10	-9	23	30
10	-11	11	16

K = 15

H	L	FOBS	FCALC
0	1	37	42
0	2	23	26
0	3	28	32
0	5	30	38
0	6	21	26
0	7	34	39
0	9	31	40
0	11	20	23
0	13	17	22
1	1	46	44
1	4	24	29
1	5	60	78
1	6	30	37
1	9	26	29
1	13	20	27
1	-1	29	32
1	-3	49	45
*1	-4	24	3
1	-7	32	41
1	-10	19	20
1	-11	40	43
1	-13	14	7
1	-14	19	20
2	0	23	29
2	1	54	57
2	4	22	29
2	5	47	50
2	9	29	27
2	-2	23	26
2	-3	52	56
*2	-5	23	11
2	-7	39	36
2	-11	30	31
3	0	24	29
3	1	41	41
3	4	34	36
3	5	40	41
3	6	19	22
3	7	23	25
3	9	27	34
3	11	19	23
3	-1	33	29
3	-3	31	33
3	-4	31	35
3	-5	31	31
3	-7	35	44
3	-8	28	33
3	-11	29	39
3	-13	11	5
4	1	38	37
4	3	39	39
4	4	24	29
4	7	30	25
4	8	25	31
4	-1	38	36
4	-3	24	22
4	-4	26	36
4	-5	26	25
4	-7	25	30
4	-9	30	37
4	-11	23	30
4	-12	17	29
4	-13	15	17
5	3	40	49
5	7	24	29
5	-1	35	38
5	-5	33	36
5	-9	26	33
5	-13	26	36
6	2	19	26
6	3	29	27
6	6	17	17
6	7	31	35
6	-1	33	42
6	-5	40	46
6	-6	20	21
6	-9	31	37
6	-13	14	27
7	1	15	21
7	2	23	25
7	3	25	28
7	4	23	13
7	5	21	20
7	6	15	21
7	-1	29	33
7	-2	18	21
7	-3	18	21
7	-5	30	33
7	-7	31	31
7	-9	22	26
7	-10	18	20
7	-13	17	28
8	0	29	10
8	1	31	33
8	2	14	22
8	-1	24	25
8	-2	24	31
8	-3	28	32
8	-6	14	14
8	-7	23	25
8	-11	14	32
9	0	11	11
9	1	20	34
9	-3	24	27
9	-4	14	21
9	-7	32	37

K = 16

H	L	FOBS	FCALC
0	0	28	37
0	1	28	33
0	3	25	23
0	4	20	25
0	8	24	32
0	12	12	21
1	3	37	40
1	4	21	28
1	7	18	36
1	8	17	21
1	11	19	24
1	-1	28	33
1	-3	27	45
1	-4	32	36
1	-5	33	36
1	-9	17	24
2	0	34	34
2	3	38	42
2	4	19	19
2	6	27	29
2	7	31	31
2	8	22	20
2	-1	30	45
2	-2	29	26
2	-5	28	65
2	-8	25	29
2	-9	27	26
2	-10	15	22
2	-12	11	16
3	1	19	16
3	2	32	37
3	3	37	30
3	5	17	16
3	6	16	26
3	9	14	18
3	-1	24	20
3	-2	32	36
3	-5	30	45
3	-6	26	30
3	-7	17	19
3	-9	22	22
3	-10	18	25
4	1	20	22
4	5	29	31
4	6	20	25
4	7	21	23
4	-1	21	21
4	-2	42	51
4	-3	21	25
4	-4	16	22
4	-7	27	24
4	-10	15	21
4	-11	17	23
5	1	28	38
5	2	18	23
5	5	24	26
5	-3	22	28
5	-6	17	19
5	-7	29	39
5	-8	15	23
5	-11	16	14
6	0	17	15
6	1	21	25
6	4	24	31
6	5	23	28
6	-2	19	25
6	-3	20	31
6	-4	20	21
6	-7	19	36
6	-11	15	21
7	0	23	36
7	1	15	23
7	-1	17	15
7	-3	17	19
7	-4	17	22
7	-5	14	14
7	-7	16	21
7	-8	17	27
7	-9	11	23
8	-1	14	25
8	-3	12	27
8	-4	17	32
8	-5	22	31
8	-6	11	17

K = 17

H	L	FOBS	FCALC
0	1	21	28
0	2	17	38
0	9	16	33
1	1	29	29
1	2	26	26
1	3	20	19
1	6	21	24
1	-1	18	14
1	-2	22	28
1	-3	22	31
1	-6	16	31
2	0	34	24
2	1	27	26
2	2	20	27
2	3	25	34
2	8	14	24
2	-2	17	22
2	-3	32	38
2	-4	23	26
2	-6	21	26
2	-7	14	11
2	-8	13	19
3	0	31	41
3	1	22	27
3	2	15	14
3	4	21	25
3	5	18	28
3	6	11	9
3	7	15	24
3	-3	19	29
3	-4	33	40
3	-5	10	7
3	-7	21	19
3	-8	17	19
3	-9	10	16
4	0	28	34
4	1	16	12
4	3	23	25
4	4	26	25
4	-2	18	3
4	-4	23	35
4	-5	26	40
4	-7	14	20
4	-8	18	27
4	-9	15	21
5	0	16	23
5	2	14	20
5	3	22	27
5	-1	16	24
5	-2	13	17
5	-4	13	16
5	-5	13	21
6	0	12	5
6	-1	16	16
6	-2	13	17
6	-5	19	26
6	-6	11	27

K = 18

H	L	FOBS	FCALC
0	4	19	33
1	0	21	24
1	4	15	27
1	-1	13	22
1	-2	13	19
1	-4	19	28
2	0	21	11
2	2	20	21
2	3	12	20
2	4	19	28
2	-1	19	17
2	-2	15	24
2	-6	15	17
3	0	10	16
3	1	16	18
3	2	21	28
*3	3	7	29
3	-1	10	15
3	-2	32	41
4	-1	9	11

TABLE III. Fractional Atomic Co-ordinates.

	Atom	x/*a*	y/*b*	z/*c*
	Ba	0.07097(8)[a]	0.22761(8)	0.37695(6)
DA_1	O_1	0.2446(12)	0.1982(11)	0.3230(8)
	O_2	0.2082(11)	0.3736(9)	0.3626(7)
	N	0.3730(12)	0.2981(11)	0.3908(8)
	C_1	0.3387(15)	0.2142(14)	0.3541(10)
	C_2	0.3048(16)	0.3753(14)	0.3889(10)
	C_3	0.4289(18)	0.1512(16)	0.3563(12)
	C_4	0.3663(19)	0.4591(18)	0.4256(13)
DA_2	O_1	0.2405(12)	0.1172(11)	0.4627(8)
	O_2	0.2158(10)	0.2948(10)	0.5120(7)
	N	0.3289(13)	0.1776(13)	0.5750(9)
	C_1	0.3080(16)	0.1119(15)	0.5198(11)
	C_2	0.2816(15)	0.2625(16)	0.5666(10)
	C_3	0.3877(18)	0.0304(16)	0.5434(12)
	C_4	0.3128(22)	0.3214(21)	0.6380(15)
DA_3	O_1	–0.0101(13)	0.1857(11)	0.4868(8)
	O_2	–0.0394(12)	0.3638(11)	0.4318(8)
	N	–0.1577(13)	0.2840(14)	0.4710(9)
	C_1	–0.1007(20)	0.2005(17)	0.4897(12)
	C_2	–0.1232(17)	0.3615(15)	0.4442(10)
	C_3	–0.1600(26)	0.1241(25)	0.5170(18)
	C_4	–0.1963(17)	0.4437(15)	0.4344(11)
DA_4	O_1	–0.1487(10)	0.1908(9)	0.3248(7)
	O_2	–0.0703(11)	0.3472(9)	0.2723(7)
	N	–0.2518(11)	0.3032(10)	0.2510(7)
	C_1	–0.2354(14)	0.2184(14)	0.2858(9)
	C_2	–0.1698(16)	0.3647(14)	0.2468(10)
	C_3	–0.3375(19)	0.1642(17)	0.2717(12)
	C_4	–0.2174(17)	0.4497(16)	0.2030(11)
DA_5	O_1	0.0091(10)	0.0410(9)	0.3591(7)
	O_2	0.0181(11)	0.1477(10)	0.2439(7)
	N	–0.0812(12)	0.0135(11)	0.2388(8)
	C_1	–0.0543(15)	–0.0040(13)	0.3125(10)
	C_2	–0.0355(15)	0.0845(14)	0.2088(10)
	C_3	–0.1175(20)	–0.0871(19)	0.3258(13)
	C_4	–0.0505(21)	0.0734(20)	0.1277(15)
$ClO_4(1)$	Cl	–0.5013(4)	0.4117(4)	0.2624(3)
	O_1	–0.4751(13)	0.3676(12)	0.2032(9)
	O_2	–0.4473(18)	0.4991(18)	0.2720(12)
	O_3	–0.4466(14)	0.3621(13)	0.3288(9)
	O_4	–0.6167(14)	0.4132(13)	0.2465(9)
$ClO_4(2)$	Cl	–0.3833(4)	0.2712(5)	0.5549(3)
	O_1	–0.3850(14)	0.2947(13)	0.4827(10)
	O_2	–0.4024(19)	0.1764(19)	0.5639(13)
	O_3	–0.2805(14)	0.3014(13)	0.6034(10)
	O_4	–0.4692(16)	0.3214(15)	0.5698(11)

[a] The quantities enclosed in brackets are the estimated standard deviations.

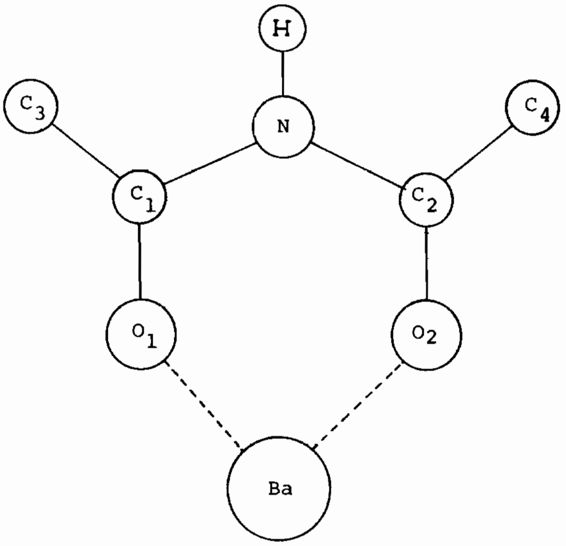

Figure 1. Atom designation for diacetamide (DA) ligands.

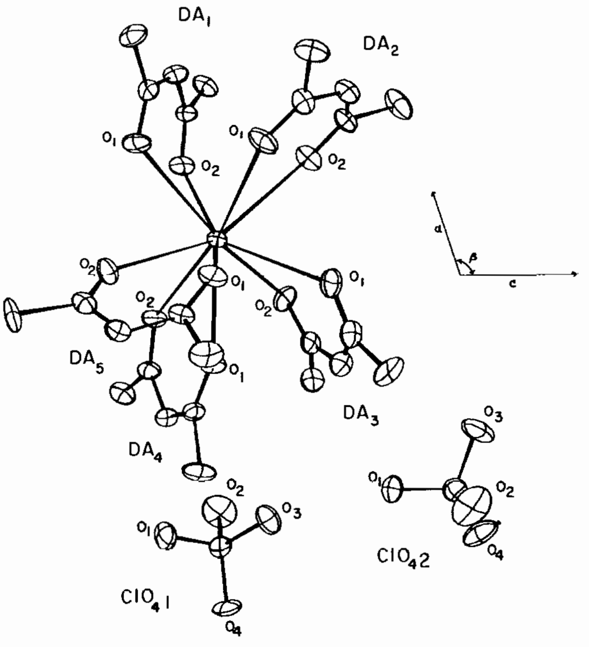

Figure 2. Projection of the asymmetric unit down the *b*-axis and on the *ab*-plane.

in Table VI. All bond angles are found in Table VII and dihedral angles between best fit planes[21] listed in Table VIII. A three-dimensional ORTEP[22] program plot of the asymmetric unit projected down the *b*-axis is shown in Figure 2. A packing diagram, Figure 3, shows the contents of the unit cell. Figure 4 is a view of the co-ordination polyhedron.

TABLE IV. Anisotropic Thermal Parameters[a] as Mean Square Amplitude (A^2).

	Atom	$U_{11} \times 10^3$	$U_{22} \times 10^3$	$U_{33} \times 10^3$	$U_{13} \times 10^3$
	Ba	34(5)[b]	30(4)	28(6)	7(9)
DA$_1$	O$_1$	47(10)	65(11)	98(10)	32(22)
	O$_2$	53(9)	40(8)	77(8)	22(19)
	N	47(9)	38(9)	71(10)	54(19)
	C$_1$	59(11)	17(13)	56(12)	57(22)
	C$_2$	33(12)	56(12)	60(12)	19(25)
	C$_3$	67(16)	62(16)	95(15)	86(32)
	C$_4$	110(18)	13(18)	137(17)	63(35)
DA$_2$	O$_1$	76(10)	56(10)	71(12)	–29(22)
	O$_2$	79(9)	25(9)	68(10)	–19(19)
	N	72(11)	35(12)	66(12)	10(22)
	C$_1$	76(13)	27(13)	56(14)	35(25)
	C$_2$	72(11)	25(12)	50(12)	–16(22)
	C$_3$	65(16)	25(16)	114(15)	3(28)
	C$_4$	134(22)	83(22)	73(21)	–28(41)
DA$_3$	O$_1$	107(11)	60(11)	66(12)	86(22)
	O$_2$	87(11)	55(11)	89(10)	120(22)
	N	78(11)	45(13)	68(12)	70(22)
	C$_1$	101(17)	52(17)	62(15)	76(32)
	C$_2$	69(14)	44(13)	52(14)	54(25)
	C$_3$	127(28)	64(29)	210(27)	225(57)
	C$_4$	88(15)	28(14)	71(14)	54(28)
DA$_4$	O$_1$	49(9)	38(8)	83(8)	63(19)
	O$_2$	43(9)	49(8)	77(8)	22(16)
	N	44(9)	22(8)	64(8)	38(16)
	C$_1$	40(11)	47(12)	62(12)	44(22)
	C$_2$	40(13)	53(13)	68(12)	22(25)
	C$_3$	46(17)	41(17)	13(17)	6(35)
	C$_4$	81(15)	36(15)	77(15)	0(28)
DA$_5$	O$_1$	53(9)	33(8)	79(10)	6(19)
	O$_2$	79(10)	52(10)	44(10)	10(19)
	N	54(10)	39(10)	64(10)	25(19)
	C$_1$	41(11)	26(11)	64(12)	6(22)
	C$_2$	50(12)	39(12)	56(12)	10(22)
	C$_3$	77(18)	38(19)	126(17)	57(35)
	C$_4$	150(22)	86(20)	27(19)	32(41)
ClO$_4$(1)	Cl	54(3)	53(3)	66(3)	41(6)
	O$_1$	89(12)	113(13)	68(12)	51(25)
	O$_2$	172(20)	60(21)	174(19)	73(38)
	O$_3$	106(14)	103(14)	66(14)	–6(25)
	O$_4$	33(14)	137(14)	120(14)	60(25)
ClO$_4$(2)	Cl	68(3)	57(3)	73(3)	41(6)
	O$_1$	96(14)	162(16)	62(14)	76(29)
	O$_2$	214(22)	19(23)	222(21)	282(41)
	O$_3$	68(14)	115(15)	98(14)	–70(29)
	O$_4$	86(16)	112(17)	181(15)	206(32)

[a] The form of the anisotropic thermal parameter is $\exp-[2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}l^2c^{*2} + 2U_{13}hla^*c^*\cos\beta^*)]$.

[b] The quantities enclosed in brackets are the estimated standard deviations.

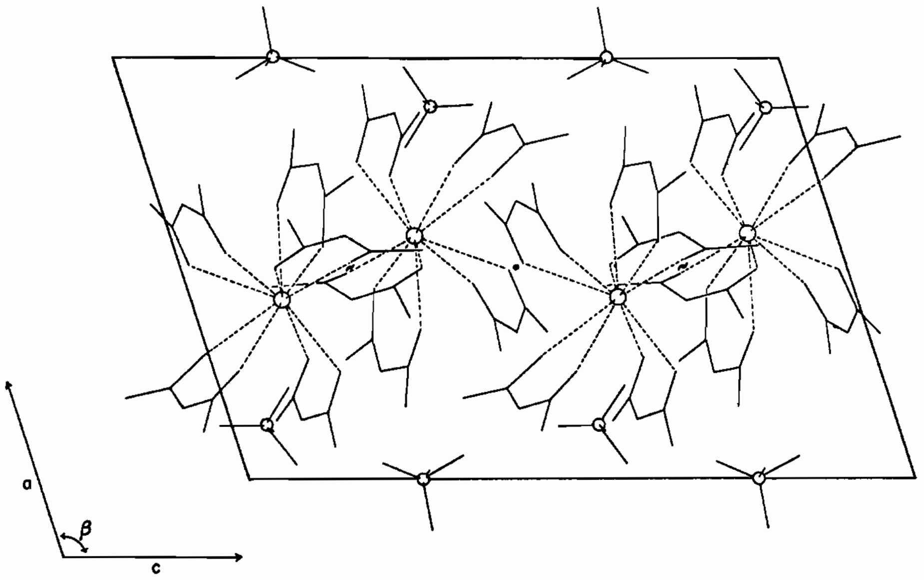

Figure 3. Packing diagram.

TABLE V. Bond Distances (A).

DA$_1$	Ba–O$_1$(2)[a]	2.80(2)[b]
	Ba–O$_2$(6)	2.82(2)
	C$_1$–O$_1$(2)	1.21(3)
	C$_2$–O$_2$(6)	1.21(3)
	C$_1$–N	1.40(3)
	C$_2$–N	1.41(3)
	C$_1$–C$_3$	1.48(3)
	C$_2$–C$_4$	1.50(4)
DA$_2$	Ba–O$_1$(1)	2.83(2)
	Ba–O$_2$(3)	2.91(2)
	C$_1$–O$_1$(1)	1.21(3)
	C$_2$–O$_2$(3)	1.23(3)
	C$_1$–N	1.38(3)
	C$_2$–N	1.38(3)
	C$_1$–C$_3$	1.55(3)
	C$_2$–C$_4$	1.54(4)
DA$_3$	Ba–O$_1$(4)	2.73(2)
	Ba–O$_2$(7)	2.84(2)
	C$_1$–O$_1$(4)	1.17(3)
	C$_2$–O$_2$(7)	1.19(3)
	C$_1$–N	1.41(3)
	C$_2$–N	1.38(3)
	C$_1$–C$_3$	1.53(5)
	C$_2$–C$_4$	1.49(4)
DA$_4$	Ba–O$_1$(8)	2.79(2)
	Ba–O$_2$(10)	2.89(2)
	C$_1$–O$_1$(8)	1.23(2)
	C$_2$–O$_2$(10)	1.25(3)
	C$_1$–N	1.40(3)
	C$_2$–N	1.40(3)
	C$_1$–C$_3$	1.51(3)
	C$_2$–C$_4$	1.49(3)
DA$_5$	Ba–O$_1$(5)	2.81(2)
	Ba–O$_2$(9)	2.74(2)
	C$_1$–O$_1$(5)	1.22(3)
	C$_2$–O$_2$(9)	1.23(3)
	C$_1$–N	1.35(3)
	C$_2$–N	1.39(3)
	C$_1$–C$_3$	1.51(4)
	C$_2$–C$_4$	1.56(4)
ClO$_4$(1)	Cl–O$_1$	1.44(2)
	Cl–O$_2$	1.43(3)
	Cl–O$_3$	1.47(2)
	Cl–O$_4$	1.45(2)
ClO$_4$(2)	Cl–O$_1$	1.44(3)
	Cl–O$_2$	1.43(3)
	Cl–O$_3$	1.46(3)
	Cl–O$_4$	1.44(3)

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[a] The numbers in brackets are in accordance with the numbering rules for co-ordination polyhedra[23]. [b] The quantities enclosed in brackets are the estimated standard deviations.

TABLE VI. Non-Bonding Interatomic Distances (A).

DA_1	Ba·····N	3.99(2)[b]	N(DA_1)·····O_3(ClO_4(1))	3.10(2)
	O_1(2)[a]·····O_2(6)	2.71(2)	N(DA_2)·····O_1(ClO_4(1))	3.06(2)
			N(DA_3)·····O_1(ClO_4(2))	3.05(2)
DA_2	Ba·····N	4.35(3)	N(DA_4)·····O_1(ClO_4(1))	2.93(2)
	O_1(1)·····O_2(3)	2.79(3)		
DA_3	Ba·····N	4.03(2)		
	O_1(4)·····O_2(7)	2.75(3)		
DA_4	Ba·····N	4.33(3)		
	O_1(8)·····O_2(10)	2.77(2)		
DA_5	Ba·····N	4.18(2)		
	O_1(5)·····O_2(9)	2.77(2)		

[a] The numbers in brackets are in accordance with the numbering rules for co-ordination polyhedra[23].

[b] The quantities enclosed in brackets are the estimated standard deviation.

TABLE VII. Bond Angles.

		Degree			Degree
DA_1	Ba–O_1(2)[a]–C_1	126.5(5)[b]	DA_3	Ba–O_1(4)–C_1	127.2(5)
	Ba–O_2(6)–C_2	126.9(5)		Ba–O_2(7)–C_2	131.5(5)
	O_1(2)–C_1–N	122.1(5)		O_1(4)–C_1–N	127.6(5)
	O_2(6)–C_2–N	123.9(5)		O_2(7)–C_2–N	121.9(5)
	O_1(2)–C_1–C_3	124.0(5)		O_1(4)–C_1–C_3	122.2(3)
	O_2(6)–C_2–C_4	123.9(5)		O_2(7)–C_2–C_4	122.0(5)
	C_3–C_1–N	113.9(5)		C_3–C_1–N	110.3(5)
	C_4–C_2–N	112.1(6)		C_4–C_2–N	116.0(6)
	C_1–N–C_2	124.4(6)		C_1–N–C_2	124.2(6)
	O_1(2)–Ba–O_2(6)	57.8(5)		O_1(4)–Ba–O_2(7)	59.3(6)
DA_2	Ba–O_1(1)–C_1	143.5(5)	DA_4	Ba–O_1(8)–C_1	145.8(5)
	Ba–O_2(3)–C_2	139.4(5)		Ba–O_2(10)–C_2	141.0(5)
	O_1(1)–C_1–N	126.6(5)		O_1(8)–C_1–N	123.7(5)
	O_2(3)–C_2–N	126.2(5)		O_2(10)–C_2–N	123.0(5)
	O_1(1)–C_1–C_3	123.2(5)		O_1(8)–C_1–C_3	124.3(5)
	O_2(3)–C_2–C_4	120.8(5)		O_2(10)–C_2–C_4	125.4(5)
	C_3–C_1–N	109.8(5)		C_3–C_1–N	112.0(5)
	C_4–C_2–N	112.9(6)		C_4–C_2–N	111.5(6)
	C_1–N–C_2	123.7(6)		C_1–N–C_2	125.9(6)
	O_1(1)–Ba–O_2(3)	58.2(6)		O_1(8)–Ba–O_2(10)	58.4(5)
DA_5	Ba–O_1(5)–C_1	133.9(5)	ClO_4(1)	O_1–Cl–O_2	106.0(5)
	Ba–O_2(9)–C_2	141.1(5)		O_1–Cl–O_3	108.9(5)
	O_1(5)–C_1–N	127.1(5)		O_1–Cl–O_4	108.7(5)
	O_2(9)–C_2–N	123.5(5)		O_2–Cl–O_3	102.8(7)
	O_1(5)–C_1–C_3	122.3(5)		O_2–Cl–O_4	117.2(6)
	O_2(9)–C_2–C_4	121.4(5)		O_3–Cl–O_4	112.8(6)
	C_3–C_1–N	110.6(5)			
	C_4–C_2–N	115.1(6)	ClO_4(2)	O_1–Cl–O_2	114.2(5)
	C_1–N–C_2	124.5(6)		O_1–Cl–O_3	108.0(6)
	O_1(5)–Ba–O_2(9)	59.9(5)		O_1–Cl–O_4	107.3(6)
				O_2–Cl–O_3	110.8(5)
				O_2–Cl–O_4	106.3(5)
				O_3–Cl–O_4	110.1(6)

[a] The numbers in brackets are in accordance with the numbering rules for co-ordination polyhedra[23].

[b] The quantities enclosed in brackets are the estimated standard deviations.

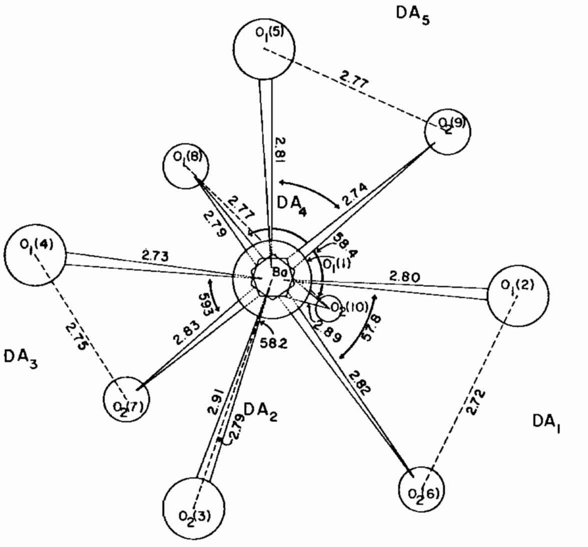

Figure 4. Projection of the co-ordination sphere down a line joing the apex (1) position and the barium atom. Ba–O and $O_1 \cdots\cdots O_2$ distances are recorded in angstrom, O_1–Ba–O_2 angles are recorded in degrees.

TABLE VIII. Planes of Best Fit and Deviations Therefrom.[a]

Plane (1) DA_1
$O_1,O_2,N,C_1,C_2,C_3,C_4$
$0.365X + 0.350Y - 0.862Z = -3.725$
Deviation (A) from plane
O_1 0.016, O_2 0.007, N –0.101,
C_1 –0.020, C_2 –0.002, C_3 0.052,
C_4 0.047
Distance (A) of other atoms from plane Ba –1.645

Plane (2) DA_2
$O_1,O_2,N,C_1,C_2,C_3,C_4$
$0.848X + 0.411Y - 0.336Z = -1.736$
Deviation (A) from plane
O_1 –0.110, O_2 0.114, N –0,037,
C_1 –0.036, C_2 0.044, C_3 0.099,
C_4 –0.072
Distance (A) of other atoms from plane Ba –0.369

Plane (3) DA_3
$O_1,O_2,N,C_1,C_2,C_3,C_4$
$-0.151X - 0.329Y - 0.932Z =$
-8.798
Deviation (A) from plane
O_1 –0.065, O_2 0.054, N 0.021,
C_1 –0.004, C_2 0.026, C_3 0.026,
C_4 –0.058
Distance (A) of other atoms from plane Ba 1.383

Plane (4) DA_4
$O_1,O_2,N,C_1,C_2,C_3,C_4$
$0.356X - 0.459Y - 0.814Z = -7.442$

TABLE VIII. (Cont.)

Deviation (A) from plane
O_1 –0.18, O_2 0.127, N –0.057,
C_1 –0.021, C_2 –0.010, C_3 0.107,
C_4 –0.038
Distance (A) of other atoms from plane Ba –0.231

Plane (5) DA_5
$O_1,O_2,N,C_1,C_2,C_3,C_4$
$-0.830X + 0.555Y - 0.052Z = 1.811$
Deviations (A) from plane
O_1 –0.069, O_2 0.134, N 0.116,
C_1 –0.025, C_2 0.071, C_3 0.047,
C_4 –0.174
Distance (A) of other atoms from plane Ba 0.724

Plane (6) DA_1
O_1,N,C_1,C_3
$0.361X + 0.413Y - 0.837Z = -3.385$
Deviation (A) from plane
O_1 0.003, N 0.003, C_1 –0.009,
C_3 0.003

Plane (7) DA_1
O_2,N,C_2,C_4
$0.391X + 0.293Y - 0.872Z = -4.075$
Deviation (A) from plane
O_2 –0.004, N –0.003, C_2 0.010,
C_4 –0.003

Plane (8) DA_2
O_1,N,C_1,C_3
$0.799X + 0.465Y - 0.382Z = -2.176$
Deviation (A) from plane
O_1 0.002, N 0.001, C_1 –0.005,
C_3 0.001

Plane (9) DA_2
O_2,N,C_2,C_4
$0.881X + 0.395Y - 0.260Z = -0.967$
Deviation (A) from plane
O_2 –0.009, N –0.008, C_2 0.022,
C_4 –0.006

Plane (10) DA_3
O_1,N,C_1,C_3
$-0.108X - 0.334Y - 0.937Z =$
-9.043
Deviation (A) from plane
O_1 –0.002, N –0.002, C_1 0.006,
C_3 –0.002

Plane (11) DA_3
O_2,N,C_2,C_4
$-0.190X - 0.300Y - 0.935Z =$
-8.493
Deviation (A) from plane
O_2 –0.005, N –0.004, C_2 0.012,
C_4 –0.003

TABLE VIII. (Cont.)

Plane (12) DA_4
O_1,N,C_1,C_3
$0.439X - 0.424Y - 0.792Z = -7.639$
Deviation (A) from plane
O_1 −0.003, N −0.002, C_1 0.007, C_3 −0.002

Plane (13) DA_4
O_2,N,C_2,C_4
$0.279X - 0.455Y - 0.846Z = -7.27$
Deviation (A) from plane
O_2 0.010, N 0.008, C_2 −0.024, C_4 0.007

Plane (14) DA_5
O_1,N,C_1,C_3
$0.793X - 0.606Y - 0.059Z = -2.237$
Deviation (A) from plane
O_1 −0.002, N −0.001, C_1 0.004, C_3 −0.001

Plane (15) DA_5
O_2,N,C_2,C_4
$-0.817X + 0.544Y - 0.191Z = 1.282$
Deviation (A) from plane
O_2 −0.009, N −0.007, C_2 0.023, C_4 −0.007

Plane (16) DA_1
O_1,Ba,O_2
$-0.331X + 0.177Y - 0.927Z = -5.486$

Plane (17) DA_2
O_1,Ba,O_2
$0.794X + 0.365Y - 0.486Z = -3.244$

Plane (18) DA_3
O_1,Ba,O_2
$-0.695X - 0.280Y - 0.663Z = -4.663$

Plane (19) DA_4
O_1,Ba,O_2
$0.393X - 0.551Y - 0.736Z = -7.476$

Plane (20) DA_5
O_1,Ba,O_2
$-0.950X + 0.268Y - 0.161Z = 0.982$

Plane (21) $ClO_4(1)$
O_1,Cl,O_2
$-0.639X + 0.420Y - 0.644Z = 4.523$

Plane (22) $ClO_4(1)$
O_3,Cl,O_4
$0.095X - 0.851Y - 0.517Z = -8.338$

Plane (23) $ClO_4(2)$
O_1,Cl,O_2
$-0.953X + 0.183Y - 0.241Z = 6.114$

Plane (24) $ClO_4(2)$
O_3,Cl,O_4
$0.271X + 0.704Y - 0657Z = -6.263$

TABLE VIII. (Cont.)

Dihedral angles between planes (deg.)

Plane	Plane		Plane	Plane	
(1)	(16)	42.2	(4)	(19)	7.3
(2)	(17)	9.6	(5)	(20)	19.0
(3)	(18)	35.5			
(6)	(7)	7.4	(12)	(13)	9.8
(8)	(9)	9.3	(14)	(15)	165.0(15.0)
(10)	(11)	5.1			
(21)	(22)	94.5			
(23)	(24)	88.4			

[a] Equations are expressed in the cosine form $lX + mY + nZ = p$ where X, Y and Z are cartesian co-ordinates related to the cell co-ordinates by $X = xa$, $Y = yb$, $Z = zc$.

Discussion

The barium ion in pentakis(diacetamide)barium(II) perchlorate forms a ten co-ordinated complex with diacetamide. The formation of decaco-ordination complexes was seriously suspected for the lanthanides and actinides, since the formation of ten hybrid orbitals require the utilization of *f*-orbitals[23]. To date, ten co-ordinated complexes which are known and have been characterized by X-rays include $La(OH_2)_4AH$ where H_4A is EDTA[24], D(+)-barium uridine-5′-phosphate[25], barium dithionate dihydrate[26], and calcium fumarate trihydrate[27]. The last three complexes involve bridging atoms and in all of the complexes, at least some of the ligands are ionic. The present compound, $[Ba(DA)_5](ClO_4)_2$, differs from all previous ones in that, (1) all the ligands are the same, (2) the co-ordination sphere is only slightly distorted, (3) the ligands are not bridging, and (4), all of the co-ordinate bond distances are approximately equal (2.73–2.91A), and are close to the sum of the ionic radii (Ba^{2+} = 1.35A, O^{2-} = 1.40A)[28].

The oxygen atoms in the diacetamide complex could be thought of as being located at the vertexes of a distorted symmetrically bicapped square antiprism (SBSA) of D_{4d} point group symmetry[29]. A projection of the co-ordination sphere down a line joining the apex (1) position of the SBSA and the barium atom is shown in Figure 4.

All of the diacetamide ligands are basically in the *trans–trans* configuration and identical to each other except for variations caused by packing and crowding considerations. The most significant variations occure in the barium–oxygen bond lengths (2.73–2.91A). Smaller variations (2.42–2.49A) were reported for the eight co-ordinated praseodymium complex with TTA[30] and were also attributed to steric effects.

Practically all distortions within each bidentate ligand goes back to the difference between Ba–O$_1$ and Ba–O$_2$ bond lengths, the differences being 0.03, 0.08, 0.10, 0.10, 0.07A for DA$_1$ to DA$_5$ respectively. In DA$_1$, both bond lengths are equal and a two fold symmetry about the Ba–N line is apparent, whereas in DA$_3$ and DA$_4$ the corresponding differences are reflected in the values of otherwise mirror related angles and bonds (Table V, VII). In terms of the above criteria, DA$_1$ may be considered as the model for diacetamide-B complexation in other chelates.

Definite twisting of the diacetamide ligands about a line passing through the oxygen atoms does exist. This twisting shows up as a dihedral angle between the two best fit planes (O_1,N,C_1,C_3) and (O_2,N,C_2,C_4) (Table VIII), and is a factor in causing splitting in the infrared bands as the ligands are no longer of the *trans–trans* (diacetamide-B) form but intermediate between it and the *cis–trans* form. Another factor which gives rise to splitting in the metal–carbonyl stretching absorption band is bending about the $O_1 \cdots O_2$ line. This bending shows up as a dihedral angle between the planes (O_1,O_2,N,C_1,C_2,C_3,C_4) and (O_1, Ba, O_2) (Table VIII).

The average Ba–O distance, 2.81A, is more than the sum of the ionic radii, while the average C–O distance, 1.21A, is less than that in crystalline urea (1.26A)[31]. This together with the hygroscopic nature of the crystals, indicate weak metal to oxygen bonding.

Previous infrared work[1] predicted the nonplanarity of at least one of the ligands due to the appearance of secondary band in the imide III region. It also predicted, from the splitting in the carbonyl stretching band, that one of the ten carbonyl terminals is not bonded to give a total co-ordination number of nine[1,2]. This present X-ray structure supports the non-planarity of some of the ligands, however, these non-planar diacetamide ligands are all bidentates.

The thermal parameters of the diacetamide ligands are high and in agreement with weak bonding. The carbon atoms C_1 and C_2 have low thermal parameters due to three sp^2 bonds. As expected, the methyl carbons, C_3 and C_4, have higher thermal parameters than the ring carbons. The carbonyl oxygens have higher thermal parameters than the average because of the weak metal to oxygen bonding.

The perchlorate moieties are ionic and are located between the cation clusters. Four of the five diacetamide nitrogens are hydrogen bonded to the perchlorate oxygens (2.929–3.095A) (Table VI). Hydrogen bonding was expected since it was previously reported from infrared data[1]. The perchlorate ions are significantly distorted from T_d geometry for the dihedral angle between the two tetrahedral planes are 94.5° and 88.4° (Table VIII). The fact that the thermal parameters of the perchlorate oxygens are very high is attributed to the shielding of the positive charge on the barium by the ligands clusters enabling freer movement of the oxygen atoms in the perchlorate moieties.

In determining[32] the barium bonding orbitals which could hybridize to give the ten-co-ordinate symmetrically bicapped square antiprism (D_{4d}) it was found that the combination $sp^3d^5f_{z(5z^2-3r^2)}$ is most reasonable. Other hybridization schemes such as sp^4d^5 would involve a $6p_z$ orbital which lies higher in energy than a $4f$ orbital.

Acknowledgements

This research was supported in part by the National Science Foundation under grant GU-2379, and by the Atomic Energy Commission under contract number AT-(30-1)-3675.

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