Of these six, four are second neighbors in the bridging network and are at a distance of 2.418 Å, while the other two are bridged to aluminum atoms which are not in the three columns of aluminum atoms surrounding the spiral and are at a distance of 2.587 Å. To summarize, the bridging about one spiral of hydrogen atoms includes all six aluminum atoms in the surrounding three columns and one hydrogen atom, each at a different distance along z, in each of the surrounding three spirals. The result is a completely bridged structure which is a three-dimensional network of 3c–2e $Al\cdots H\cdots Al$ bonds, consistent with the rather high observed crystalline density.

The structure is thermodynamically unstable with respect to decomposition to the elements.[25] Possibly, the layering of the hydride structure facilitates the release of H as H_2. The fact that the geometry of the Al atoms in the Al layer is the same as that in the metal,[26] except that the $Al\cdots Al$ distance in AlH_3 is 4.45 Å and in Al metal is 2.86 Å, suggests a mechanism of decomposition in which loss of H_2 is followed by a lattice contraction in the layer and a lattice expansion in the z axis direction, from 1.97 Å in the hydride to the 2.338 Å of Al metal.

Our AlH_3 structure appears to be isostructural with the essentially ionic structure of AlF_3[27] in which the $Al^{3+}\cdots F^-$ distance of 1.79 Å is slightly shorter than would be expected from the sum of ionic radii (1.86 Å). Three-center covalent bonding may be contributing to cause this shortening.

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CONTRIBUTION FROM THE DEPARTMENT OF CHEMISTRY,
UNIVERSITY OF KENTUCKY, LEXINGTON, KENTUCKY 40506

The Crystal and Molecular Structure of Ytterbium Acetylacetonate Monohydrate[1]

BY JAMES A. CUNNINGHAM,[2] DONALD E. SANDS,[3] WILLIAM F. WAGNER, AND MARY F. RICHARDSON

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The crystal structure of $Yb(C_5H_7O_2)_3(H_2O)$, tris(acetylacetonato)aquoytterbium(III), has been determined from three-dimensional X-ray diffraction data collected by counter methods. A total of 2992 independent reflections, for which the intensity exceeded 1.07 times the background, were recorded as observed. Four molecules crystallize in a triclinic unit cell of symmetry $P\bar{1}$ and dimensions a = 13.01 Å, b = 18.33 Å, c = 8.32 Å, α = 100.40°, β = 102.12°, and γ = 105.19°. The calculated and observed densities are 1.72 and 1.74 g cm^{-3}, respectively. The structure has been refined by the method of least squares to a value of 0.076 for the conventional R factor. The two crystallographically independent ytterbium ions are seven-coordinate, each being bonded to three acetylacetonate groups and one water molecule. A hydrogen bond links the independent molecules in pairs. The coordination polyhedra formed about the independent ytterbium ions may both be described as capped trigonal prisms.

Introduction

The trisacetylacetonates of the lanthanides and ytterbium form metastable trihydrates which decompose to stable monohydrates.[4] A recent study[5] has shown that the dihydrated form is not an intermediate in the dehydration of the trihydrated chelate. However, the dihydrates of the lanthanum, praseodymium, neodymium, and samarium chelates can be prepared by recrystallizing the trihydrated form from cold 95% ethanol. We have previously determined the structure of yttrium acetylacetonate trihydrate[6] and lanthanum acetylacetonate dihydrate.[7]

The monohydrated forms of yttrium, lanthanum, cerium, praseodymium, neodymium, samarium, europium, gadolinium, dysprosium, holmium, erbium, and ytterbium have been prepared and character-

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ized.[5] Powder patterns show that there are two distinct monohydrate structures. The compounds of the lower rare earths have a triclinic structure, involving dimers, which has so far defied elucidation and which may be disordered. Ytterbium acetylacetonate monohydrate is not isostructural with the monohydrated form of the chelates of the lower rare earths.

Experimental Section

An analyzed sample of the monohydrated form of ytterbium acetylacetonate, which had been prepared by the method of Stites, McCarty, and Quill[8] and recrystallized from acetylacetone,[4] was obtained.

With the aid of a polarizing microscope, a suitable crystal, with dimensions 0.18 × 0.09 × 0.09 mm, was chosen and sealed in a thin-walled glass capillary with the 0.18-mm dimension parallel to the capillary. Preliminary oscillation and Weissenberg photographs indicated the triclinic crystal system. The crystal was transferred to a General Electric **X**-ray spectrometer equipped with a single-crystal orienter and scintillation counter with a pulse height analyzer. The crystal was oriented about b^*. The triclinic diffraction symmetry was confirmed and accurate unit cell dimensions were obtained by slow θ–2θ scans; they are $a = 13.009 \pm 0.008$ Å, $b = 18.833 \pm 0.016$ Å, $c = 8.325 \pm 0.004$ Å, $\alpha = 100.395 \pm 0.043°$, $\beta = 102.118 \pm 0.095°$, and $\gamma = 105.192 \pm 0.021°$. The measured density[9] is 1.72 ± 0.02 g cm^{-3}; the calculated density for four molecules per unit cell is 1.74 g cm^{-3}.

The intensities of all of the independent reflections for which $2\theta \leq 40°$ were measured manually using a 40-sec counting period and zirconium-filtered Mo Kα radiation. Goniostat settings were calculated for the Mo Kα_1 line (λ 0.70930 Å), and conversion factors for obtaining integrated intensities were based upon 12 intensities measured by a manual ω scan. Background corrections were obtained by interpolation of a plot of background *vs.* 2θ which was based on measurements made with the crystal set out of reflecting position. Corrections for instrumental fluctuations and variations of intensity due to crystal decomposition were obtained by periodically measuring a standard reflection. A total decrease in intensity of about 10% was observed.

A total of 3496 independent reflections were measured. A total of 504 reflections, for which the intensity did not exceed 1.07 times the background and therefore could not confidently be distinguished from background with the observed counting rate, were recorded as unobserved. The intensities were converted to structure factors in the usual manner. No corrections were applied for absorption or extinction ($\mu = 53.0$ cm^{-1}). The maximum possible variation in the ratio of any two intensities due to absorption is about 21%.

Structure Determination and Refinement

Trial ytterbium positions were deduced from the three-dimensional Patterson function. Further interpretation of the Patterson map was not attempted owing to extensive crowding and overlapping of the peaks. Space group $P\bar{1}$, suggested by a negative piezoelectric test, was assumed (later confirmed by the successful refinement of the structure). The two crystallographically independent ytterbium atoms, Yb(1) and Yb(2), occupy the $P\bar{1}$ general positions 2(i): $\pm(x, y, z)$, with $x(1) = 0.37$, $y(1) = -0.24$, and $z(1) = -0.07$; and $x(2) = 0.24$, $y(2) = 0.21$, and $z(2) = 0.26$. The ytterbium positional parameters and one scale factor were refined by the method of least squares.

The contributions of neutral Yb to the observed structure factors were computed, and a difference Fourier map based on $F_o - F_c$ of the 2721 reflections for which $|F_c| > 0.40\,|F_o|$ was calculated. This difference Fourier synthesis had 13 prominent peaks at approximately the distance from the ytterbium atoms expected for oxygen atoms. Five additional peaks were found which could be attributed to the carbon atoms of one complete acetylacetonate group. Two additional difference Fourier maps were required before all of the remaining oxygen and carbon atoms could be located.

The atomic parameters and one scale factor were refined by the method of least squares using a local IBM 360 adaptation of the program of Busing, Martin, and Levy.[10] The atomic form factors included were taken from Cromer, Larson, and Waber[11] for ytterbium and from the compilation of Ibers[12] for oxygen and carbon. The contributions to the least-squares sums were weighted by $1/\sigma^2$, in which σ for each reflection was calculated by a variation of the method of Smith and Alexander,[13] which includes the contribution to the error of each correction factor, such as background measurements, conversion of peak heights to integrated intensities, and corrections for instrumental variations. Unobserved data were omitted from the refinement. Included in the refinement were the positional parameters of the 46 independent atoms, individual anisotropic temperature factors of the form $\exp[-(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})]$ for the ytterbium atoms, individual isotropic temperature factors for the oxygen and carbon atoms, and one scale factor. During the last cycle of refinement the contributions of the ytterbium atoms to the structure factors were corrected for the real and imaginary components of anomalous dispersion. The values of $\Delta f'$ and $\Delta f''$ were taken from the compilation of Templeton.[14] The final value of the residual, $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, was 0.076 for the 2992 observed data. The ytterbium contributions alone gave $R = 0.251$, and before the anomalous dispersion correction R was 0.080 for the complete structure. The mean positional parameter shift during the last least-squares cycle was 0.00098. The standard deviation of an observation of unit weight was 0.82. Hydrogen atom positions were not determined.

The magnitudes of the final observed and calculated structure factors are listed in Table I. The atomic coordinates and temperature factors are given in Table II.

Discussion of the Structure

Figure 1 shows the two crystallographically independent molecules projected along [001]. Table III

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TABLE I

MAGNITUDES OF OBSERVED AND CALCULATED FACTORS FOR OBSERVED DATA, EACH MULTIPLIED BY 10 [$10F(000) = 5720$]

H	K	FO	|FC|
L=0			
0	-1	371	319
0	-2	1881	1831
0	-3	466	420
0	-4	903	874
0	-5	661	646
0	-6	322	301
0	-7	584	565
0	-8	204	161
0	-9	727	723
0	-10	186	71
0	-11	172	139
0	-12	65	18
0	-13	130	132
0	-14	164	163
0	-15	198	186
0	-16	187	204
1	0	691	667
1	-1	241	236
1	-2	961	941
1	-3	118	121
1	-4	290	287
1	-6	675	689
1	-7	292	278
1	-8	668	651
1	-9	679	689
1	-10	506	507
1	-11	822	777
1	-12	155	191
1	-13	563	571
1	-15	376	403
1	-16	79	103
1	-17	301	286
-1	-1	177	167
-1	-2	95	73
-1	-3	215	199
-1	-4	52	26
-1	-5	128	146
-1	-6	233	246
-1	-7	464	480
-1	-8	192	161
-1	-9	499	501
-1	-10	139	145
-1	-11	615	604
-1	-12	415	376
-1	-13	459	471
-1	-14	428	420
-1	-15	276	299
-1	-16	459	472
2	0	983	996
2	-1	620	637
2	-2	643	646
2	-3	276	264
2	-4	539	546
2	-6	320	304
2	-7	185	182
2	-9	99	100
2	-10	241	253
2	-11	293	278
2	-12	302	311
2	-13	327	340
2	-14	127	139
2	-15	350	369
2	-17	338	375
-2	-1	729	751
-2	-2	606	589
-2	-3	904	866
-2	-4	107	116
-2	-5	873	909
-2	-6	317	304
-2	-7	813	775
-2	-8	475	460
-2	-9	580	554
-2	-10	441	439
-2	-11	318	307
-2	-12	314	313
-2	-13	95	84
-2	-14	201	199
3	0	213	223
3	-1	626	687
3	-2	524	541
3	-3	714	709
3	-4	1101	1063
3	-5	602	598
3	-6	1171	1146
3	-7	309	291
3	-8	1100	1071
3	-10	752	752
3	-11	340	318
3	-12	432	457
3	-13	259	282
3	-14	104	148
3	-15	142	167
3	-17	75	52
-3	-1	1004	941
-3	-2	64	98
-3	-3	539	533
-3	-4	88	68
-3	-5	320	295
-3	-6	52	13
-3	-7	45	77
-3	-10	211	225
-3	-12	259	280
-3	-14	388	397
-3	-15	128	92
4	-1	260	287
4	-4	105	51
4	-5	252	251
4	-6	647	627
4	-7	309	284
4	-8	1098	930
4	-9	110	124
4	-10	773	763
4	-12	668	632
4	-13	229	241
4	-14	457	471
4	-15	385	384
4	-16	334	362
4	-17	395	415
-4	-1	251	239
-4	-2	173	179
-4	-3	551	549
-4	-4	618	556
-4	-5	587	553
-4	-6	657	644
-4	-7	391	407
-4	-8	768	789
-4	-9	173	150
-4	-10	563	583
-4	-11	75	95
-4	-12	525	531
-4	-13	283	274
-4	-14	427	362
5	0	229	253
5	-1	892	890
5	-3	708	790
5	-4	79	117
5	-5	943	923
5	-6	220	223
5	-7	323	300
5	-8	149	173
5	-9	99	115
5	-10	149	63
5	-14	97	108
5	-15	84	44
5	-16	336	310
5	-17	141	135
-5	-1	872	862
-5	-2	749	746
-5	-3	198	637
-5	-4	787	846
-5	-5	281	240
-5	-6	438	438
-5	-7	117	135
-5	-8	356	366
-5	-9	58	54
-5	-10	130	136
-5	-11	110	113
-5	-12	86	57
-5	-13	140	83
6	0	343	318
6	-1	121	152
6	-2	122	136
6	-3	242	313
6	-4	109	99
6	-5	758	742
6	-6	212	119
6	-7	859	840
6	-8	285	263
6	-9	618	594
6	-10	429	419
6	-11	527	484
6	-12	437	419
6	-13	247	237
6	-14	554	572
6	-16	538	487
6	-17	84	119
-6	-1	153	120
-6	-2	383	356
-6	-4	184	165
-6	-6	337	325
-6	-7	106	85
-6	-8	411	401
-6	-9	219	198
-6	-10	261	271
-6	-11	250	264
-6	-12	167	179
7	0	553	550
7	-1	240	235
7	-2	497	475
7	-3	409	391
7	-4	332	323
7	-5	393	373
7	-7	157	104
7	-8	66	88
7	-9	153	172
7	-11	384	371
7	-12	242	246
7	-13	315	303
7	-14	325	332
7	-15	311	267
7	-16	624	563
7	-17	166	121
-7	-1	84	100
-7	-2	714	693
-7	-4	710	723
-7	-5	274	293
-7	-6	582	583
-7	-7	493	450
-7	-8	415	391
-7	-9	459	440
-7	-10	175	148
8	0	629	593
8	-2	603	614
8	-3	242	260
8	-4	647	652
8	-5	479	475
8	-6	469	441
8	-7	582	550
8	-8	242	236
8	-11	403	397
8	-13	211	214
8	-15	65	88
-8	-1	65	93
-8	-2	342	349
-8	-3	119	129
-8	-4	170	194
-8	-8	123	21
-8	-9	69	74
9	0	221	197
9	-1	107	87
9	-4	194	187
9	-6	191	191
9	-7	181	195
9	-8	225	222
9	-9	373	352
9	-10	266	243
9	-11	490	465
9	-12	150	170
9	-13	566	528
9	-15	492	451
-9	-1	234	244
-9	-2	153	174
-9	-3	287	305
-9	-4	143	161
-9	-5	375	344
-9	-7	445	395
10	0	402	354
10	-1	449	423
10	-2	603	562
10	-3	264	255
10	-4	464	438
10	-5	73	75
10	-6	292	307
10	-8	186	162
10	-10	76	73
-10	-1	383	378
-10	-2	212	214
-10	-3	455	460
-10	-5	387	353
11	0	174	101
11	-1	151	154
11	-2	222	206
11	-3	352	349
11	-4	340	317
11	-5	161	148
11	-6	226	246
11	-8	355	349
11	-10	434	382
11	-11	196	171
11	-12	446	423
-11	-1	146	83
12	-2	114	68
12	-3	163	143
12	-4	65	56
L=1			
0	0	636	611
0	1	1227	1216
0	2	601	584
0	3	459	456
0	4	1347	1240
0	5	199	146
0	6	960	1000
0	7	215	189
0	8	925	924
0	9	350	286
0	10	629	631
0	11	216	204
0	12	234	255
0	13	70	144
0	-1	1273	1275
0	-2	212	203
0	-3	764	739
0	-4	75	80
0	-5	999	949
0	-6	320	321
0	-7	146	120
0	-8	271	291
0	-9	69	36
0	-10	113	135
0	-11	197	174
0	-12	474	488
0	-13	142	82
0	-14	437	464
0	-16	378	409
0	-17	199	169
1	0	790	789
1	1	145	167
1	2	55	70
1	3	247	232
1	4	552	525
1	6	142	146
1	7	140	156
1	10	168	179
1	11	415	389
1	12	175	166
1	13	421	431
1	14	104	55
1	15	407	428
1	-1	795	805
1	-2	785	795
1	-3	989	985
1	-4	104	97
1	-5	1662	1754
1	-6	139	135
1	-7	1041	1049
1	-8	116	165
1	-9	820	795
1	-10	288	293
1	-11	499	504
1	-12	310	321
1	-13	166	201
1	-14	272	295
1	-16	117	149
-1	0	158	136
-1	1	171	179
-1	2	105	70
-1	3	163	130
-1	4	108	77
-1	5	444	440
-1	6	527	515
-1	7	395	417
-1	8	343	350
-1	9	199	191
-1	10	730	703
-1	11	210	157
-1	12	743	726
-1	13	329	344
-1	14	519	535
-1	15	366	384
-1	16	293	318
-1	-1	861	886
-1	-2	277	282
-1	-3	503	498
-1	-4	314	315
-1	-5	570	574
-1	-6	414	446
-1	-7	655	655
-1	-8	655	636
-1	-9	410	434
-1	-10	688	670
-1	-11	97	100
-1	-12	700	681
-1	-13	215	156
-1	-14	501	508
-1	-15	312	306
-1	-16	322	328
2	0	459	466
2	1	109	106
2	2	626	630
2	3	174	206
2	4	672	693
2	5	554	561
2	6	678	677
2	7	726	719
2	8	482	463
2	9	584	596
2	10	235	250
2	11	568	587
2	13	434	470
2	14	121	111
2	15	327	308
2	-1	93	91
2	-2	367	368
2	-3	182	354
2	-4	307	306
2	-5	250	263
2	-6	120	114
2	-7	513	523
2	-8	95	95
2	-9	438	424
2	-11	707	706
2	-12	274	281
2	-13	532	540
2	-14	338	375
2	-15	248	296
2	-16	332	351
2	-17	147	179
-2	0	494	516
-2	1	1418	1472
-2	2	230	215
-2	3	897	871
-2	4	162	170
-2	5	608	590
-2	6	428	412
-2	7	346	335
-2	8	421	410
-2	9	176	185
-2	10	260	248
-2	12	79	95
-2	13	99	94
-2	14	206	227
-2	15	145	148
-2	16	226	221
-2	17	129	133
-2	-1	1480	1582
-2	-2	533	544
-2	-3	944	949
-2	-4	700	714
-2	-5	371	356
-2	-6	782	779
-2	-8	440	446
-2	-9	128	97
-2	-10	279	258
-2	-11	78	75
-2	-12	67	76
-2	-13	69	68
-2	-15	139	111
-2	-16	150	148
3	0	1176	1222
3	1	245	261
3	2	908	922
3	3	548	545
3	4	715	687
3	5	641	645
3	6	371	377
3	7	407	423
3	8	109	132
3	9	231	249
3	14	90	89
3	-2	1274	1257
3	-3	327	332
3	-4	983	981
3	-5	456	477
3	-6	743	715
3	-7	626	593
3	-8	435	417
3	-9	619	570
3	-10	130	143
3	-11	352	348
3	-13	65	49
3	-15	207	209
3	-16	109	137
3	-17	165	206
3	-18	141	171
-3	0	70	32
-3	1	192	142
-3	2	95	101
-3	3	1072	963
-3	4	112	95
-3	5	964	985
-3	6	168	191
-3	7	989	987
-3	8	445	458
-3	9	753	758
-3	10	651	670
-3	11	472	484
-3	12	751	792
-3	13	153	148
-3	14	513	559
-3	16	382	379
-3	17	68	106
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3	-16	134	107
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4	-8	431	438
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5	8	546	496
5	9	108	123
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5	-2	94	84
5	-3	266	230
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-5	14	521	529
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-5	-1	81	17
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-5	-5	244	211
-5	-6	522	532
-5	-7	98	58
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-5	-9	95	70
-5	-10	503	479
-5	-11	207	217
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6	3	124	122
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6	7	143	172
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6	-2	307	316
6	-3	568	530
6	-4	212	203
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7	-4	362	354
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7	-6	239	252
7	-7	556	556
7	-9	386	367
7	-10	71	121
7	-11	357	413
7	-12	168	222
7	-13	206	212
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7	-15	130	122
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-7	-4	83	9
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8	3	218	215
8	4	300	266
8	-7	174	199
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8	-9	387	381
8	-10	73	78
8	-11	511	468
8	-13	471	444
8	-14	196	195
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9	-6	425	362
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9	-8	199	200
9	-9	159	225
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9	-11	180	201
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-9	-1	347	373
-9	-2	350	327
-9	-3	338	337
-9	-4	217	164
-9	-5	213	182
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10	-3	226	172
10	-4	300	264
10	-6	396	350
10	-8	430	385
10	-9	204	223
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-10	-4	57	115
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-11	3	266	292
-11	4	240	236
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-11	6	202	216
-11	-1	357	357
-11	-3	388	360
-11	-4	101	105
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-12	5	323	306
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-12	7	216	213
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0	8	96	141
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0	10	244	273
0	11	168	186
0	12	264	278
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0	-2	290	278
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0	-4	114	71
0	-5	726	728
0	-6	273	254
0	-7	665	679
0	-8	442	454
0	-9	445	472
0	-10	509	524
0	-11	206	219
0	-12	498	505
0	-14	275	314
0	-15	107	63
0	-16	153	150
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1	1	347	295
1	2	540	504
1	3	173	135
1	4	670	651
1	5	66	12
1	6	573	561
1	7	178	204
1	8	500	516
1	9	381	387
1	10	277	281
1	11	326	338
1	-1	521	543
1	-2	105	70
1	-3	96	39
1	-4	181	164
1	-5	71	104
1	-6	45	16
1	-7	219	225
1	-8	64	54
1	-9	243	266
1	-10	109	109
1	-11	327	331
1	-12	294	317
1	-13	281	300
1	-14	405	440
1	-15	68	71
1	-16	422	425
-1	0	111	96
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-1	2	254	254
-1	3	668	694
-1	4	426	424
-1	5	460	481
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-1	7	218	229
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2	5	169	177
2	6	240	236
2	7	269	276
2	8	121	137
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2	-3	421	414
2	-4	350	334
2	-5	409	448
2	-6	324	348
2	-7	633	654
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2	-11	385	413
2	-12	73	53
2	-17	72	46
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-2	-13	222	198
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3	3	176	184
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3	5	331	360
3	6	167	212
3	7	416	435
3	9	506	504
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3	-2	213	203
3	-3	103	43
3	-4	334	332
3	-5	254	249
3	-6	254	294
3	-7	405	495
3	-8	326	350
3	-9	572	574
3	-10	232	211
3	-11	617	613
3	-12	92	71
3	-13	526	486
3	-14	89	86
3	-15	332	324
3	-16	223	235
3	-17	198	206
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-3	5	460	456
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-3	7	186	192
-3	8	108	125
-3	11	93	81
-3	12	98	121
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-3	-2	686	702
-3	-3	436	459
-3	-4	849	875
-3	-5	151	109
-3	-6	696	704
-3	-7	202	169
-3	-8	455	425
-3	-9	219	244
-3	-10	286	280
-3	-11	107	105
-3	-12	121	67
-3	-13	110	63

contains the bond lengths and angles; the standard deviations were calculated by the method of Sands.[15] Figure 2 shows the average dimensions of an ytterbium acetylacetonate ring.

Each independent ytterbium atom is bonded to seven oxygen atoms, contributed by three bidentate acetylacetonate groups and one water molecule. Yb(1) is

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(15) D. E. Sands, *Acta Cryst.*, **21**, 868 (1966).

TABLE I (*Continued*)

H	K	FO	|FC|
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4	4	172	157
4	5	478	481
4	6	99	19
4	7	495	452
4	-1	313	268
4	-2	561	550
4	-3	145	102
4	-4	383	406
4	-5	87	83
4	-6	272	287
4	-7	90	70
4	-8	79	126
4	-12	112	104
4	-13	143	163
4	-15	270	274
4	-16	99	78
-4	0	424	453
-4	1	199	207
-4	2	282	302
-4	3	546	551
-4	4	292	283
-4	5	929	972
-4	6	149	116
-4	7	742	789
-4	9	529	558
-4	10	76	73
-4	11	258	311
-4	12	96	159
-4	13	190	238
-4	-1	177	183
-4	-2	631	684
-4	-3	125	54
-4	-4	569	588
-4	-5	175	179
-4	-6	74	11
-4	-7	98	73
-4	-8	120	133
-4	-9	94	66
-4	-10	263	237
-4	-11	254	220
-4	-12	132	105
-4	-13	321	303
5	0	246	207
5	1	232	214
5	2	72	26
5	3	83	107
5	-1	265	236
5	-2	391	366
5	-3	139	152
5	-4	477	491
5	-5	92	144
5	-6	551	590
5	-8	486	538
5	-9	213	226
5	-10	395	419
5	-11	237	254
5	-12	233	236
5	-13	249	243
5	-14	74	109
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-5	7	163	165
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-5	-3	229	219
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1	-11	176	152
-1	0	69	4
-1	1	125	64
-1	2	66	15
-1	4	109	83
-1	-1	150	132
-1	-2	60	34
-1	-3	202	196
-1	-4	158	65
-1	-5	266	288
-1	-6	201	211
-1	-7	242	303
-1	-8	324	321
-1	-9	156	128
-1	-10	349	353
-1	-11	67	50
2	0	111	101
2	-1	84	62
2	-2	76	18
2	-3	94	39
2	-4	70	112
2	-5	157	122
2	-6	69	14
2	-7	185	184
2	-9	255	266
2	-10	68	82
-2	0	206	224
-2	1	489	448
-2	2	82	31
-2	3	501	457
-2	4	158	163
-2	5	345	321
-2	-1	362	328
-2	-2	235	253
-2	-3	282	243
-2	-4	208	173
-2	-5	188	205
-2	-6	252	221
-2	-7	109	51
-2	-8	170	129
-2	-9	89	31
-2	-10	100	98
-2	-11	71	23
3	-2	405	386
3	-3	67	31
3	-4	264	256
3	-5	120	125
3	-6	160	171
3	-7	152	124
3	-8	124	126
-3	0	170	140
-3	2	127	120
-3	3	364	328
-3	4	99	75
-3	5	317	300
-3	-1	124	41
-3	-2	79	4
-3	-3	112	6
-3	-4	149	128
-3	-5	61	6
-3	-6	234	247
-3	-8	241	247
-3	-9	95	81
-3	-10	262	245
-4	0	252	228
-4	1	176	163
-4	2	162	149
-4	3	188	161
-4	4	142	112
-4	5	152	132
-4	-1	140	107
-4	-2	356	353
-4	-3	101	33
-4	-4	413	439
-4	-5	166	116
-4	-6	392	373
-4	-7	237	194
-4	-8	251	259
-4	-9	215	203
-4	-10	178	157
-5	0	312	300
-5	2	319	297
-5	3	260	202
-5	4	295	246
-5	5	316	296
-5	-1	92	33
-5	-2	268	271
-5	-3	73	54
-5	-4	162	150
-5	-5	102	65
-5	-6	68	39
-5	-7	98	28
-5	-8	91	13
-6	0	179	140
-6	1	89	49
-6	2	93	63
-6	4	88	31
-6	5	96	38
-6	-1	145	76
-6	-2	232	193
-6	-3	147	139
-6	-4	136	146
-6	-5	241	224
-6	-6	105	84
-6	-7	313	287
-7	0	434	442
-7	1	228	206
-7	2	406	374
-7	3	125	93
-7	4	359	350
-7	-1	341	335
-7	-2	259	260
-7	-3	336	302
-7	-4	108	108
-7	-5	262	277
-8	0	114	86
-8	1	147	172
-8	2	197	161
-8	-1	132	66
-8	-2	96	91
L=8			
-2	-3	117	71
-2	-4	215	209
-3	-2	133	124
-3	-3	100	55
-3	-4	163	145

bonded to the carbonyl oxygen atoms O(1-2), O(1-3), O(1-4), O(1-5), O(1-6), and O(1-7) and to the water molecule O(2-1).

The average ytterbium to carbonyl oxygen distance is some 0.10 Å shorter than the value of 2.336 Å for the average distance of ytterbium to coordinated water. The corresponding values in $Y(C_5H_7O_2)_3 \cdot 3H_2O$[6] were 2.366 and 2.409 Å, while in $La(C_5H_8O_2)_3 \cdot 2H_2O$[7] the corresponding values were 2.473 and 2.573 Å. The empirical relationship of Lingafelter and Braun,[16] based on a study of distances in acetylacetonates of metal ions having noble gas electronic configurations, predicts a value of 2.333 Å for the ytterbium to carbonyl oxygen distance. The average O–O separation in a ring, the "bite" of a ring, is 2.760 Å which compares favorably with the average value of 2.781 Å found by Lingafelter and Braun[16] in a survey of 13 acetylacetonate chelates; the average ring dimensions also compare favorably with those found in the survey.

The mean deviations of the carbon and oxygen atoms from the least-squares planes of the acetylacetonate groups are 0.056, 0.020, and 0.023 Å for the rings containing O(1-2)–O(1-3), O(1-4)–O(1-5), and O(1-6)–O(1-7), respectively. The deviations of Yb(1) from the planes are 0.19 ± 0.04, 0.59 ± 0.01, and 0.05 ± 0.01 Å, respectively. For the acetylacetonate groups bonded to Yb(2) we have 0.016, 0.014, and 0.050 Å as the mean deviations of the carbon and oxygen atoms from the least-squares planes of the rings containing O(2-2)–O(2-3), O(2-4)–O(2-5), and O(2-6)–O(2-7), respectively. The deviations of Yb(2) from the planes are 0.04 ± 0.01, 0.58 ± 0.01, and 0.35 ± 0.04 Å, respectively. The metal–chelate rings containing O(1-6)–O(1-7) and O(2-2)–O(2-3) are essentially planar; the sums of the interior angles of these rings are 719.8 and 719.9°, respectively, compared with 720° required for planarity. The four remaining metal–chelate rings are each folded about a line passing through their two oxygen atoms. The angle of folding is 19.7° for the O(1-4)–O(1-5) ring, 7.0° for the O(1-2)–O(1-3) ring, 14.0° for the O(2-4)–O(2-5) ring, and 10.1° for the O(2-6)–O(2-7) ring. The average sum of the interior angles for these four metal–chelate rings is 714.3°. The O(1-4)–O(1-5) ring is folded away from the O(1-6)–O(1-7) ring and toward the O(1-2)–O(1-3) ring. The O(1-2)–O(1-3) ring is folded toward the coordinated water molecule O(1-1). The O(2-4)–O(2-5) ring is folded away from the O(2-2)–O(2-3) ring and toward the O(2-6)–O(2-7) ring. The O(2-6)–O(2-7) ring is folded toward the coordinated water molecule O(2-1).

A hydrogen bond (27.3 Å) links the water molecule O(2-1) to the carbonyl oxygen atom O(1-6). Thus the independent molecules are linked in pairs. The shortest contact distance between pairs (3.98 Å) is the C(2-11)–C(1-6)′ distance, where the prime indicates the atom related to C(1-6) shown in Figure 1 by the center of symmetry at $^1/_2$, $^1/_2$, 0. All other contact distances between pairs are greater than 4.00 Å. Contact dis-

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(16) E. C. Lingafelter and R. L. Braun, *J. Am. Chem. Soc.*, **88**, 2951 (1966).

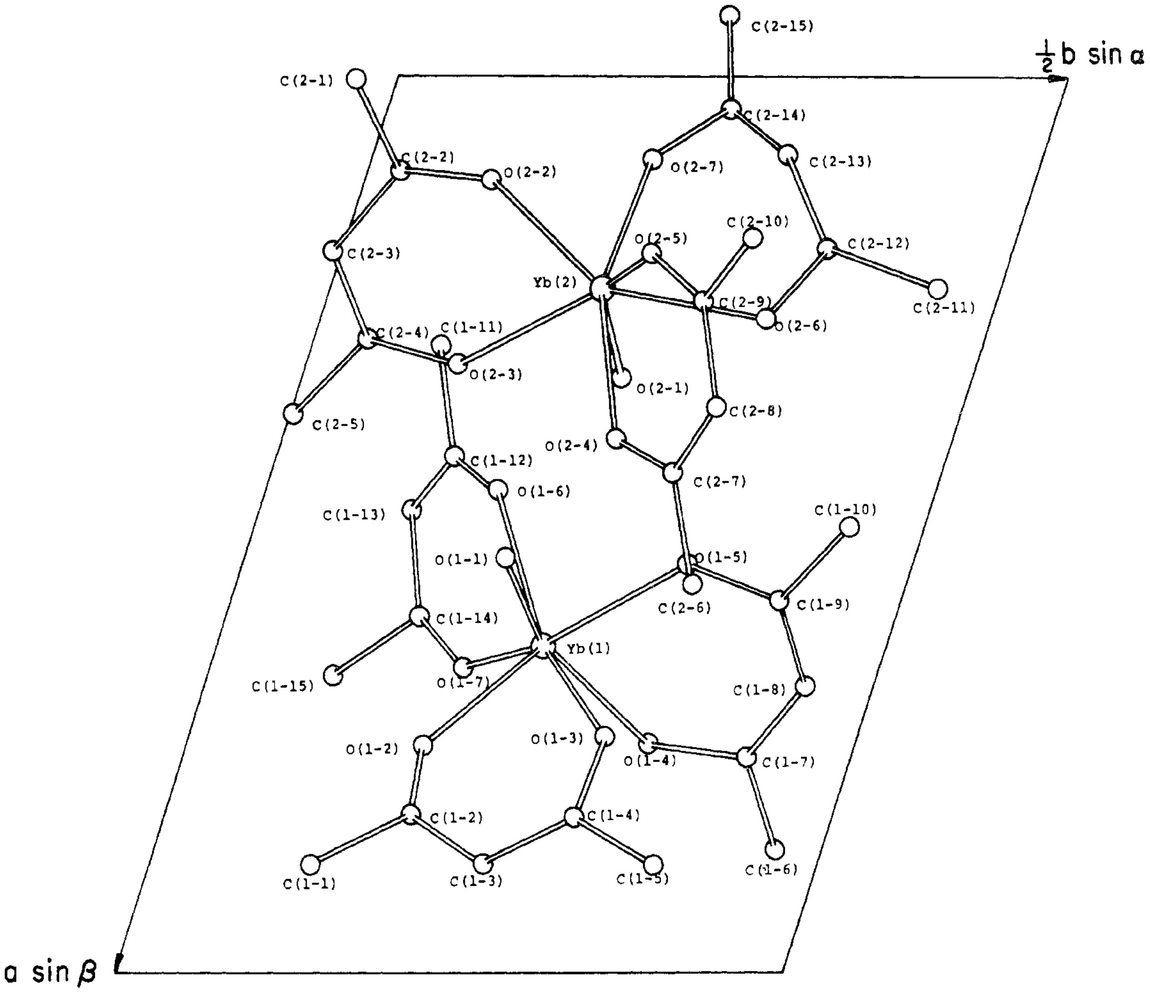

Figure 1.—Projection of the two independent molecules along [001]. Molecules shown are linked by a hydrogen bond.

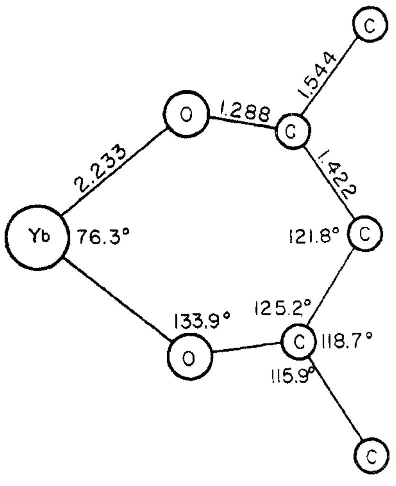

Figure 2.—Average dimensions of a ring in $Yb(C_5H_7O_2)_3 \cdot H_2O$.

tances between the molecules linked by the hydrogen bond are 3.03, 3.15, and 3.84 Å for O(1-1)–O(2-4), O(1-1)–O(2-1), and O(2-3)–C(1-11), respectively. All other contact distances are greater than 4.00 Å.

The coordination polyhedra about the crystallographically independent ytterbium atoms are shown in Figures 3 and 4. Table IV contains the distances and angles of the polyhedra.

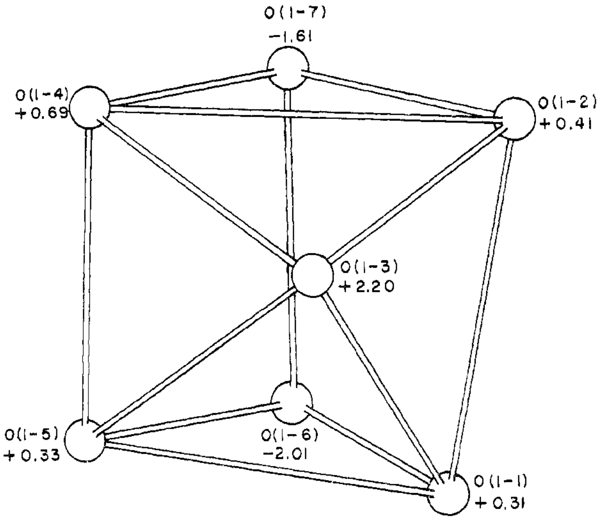

Figure 3.—Coordination polyhedron formed by the seven oxygen atoms bonded to Yb(1). The distance of each atom from the central plane is given. The view is along a vector 30° from Yb(1)–O(1-6) in the plane of Yb(1)–O(1-6)–O(1-7).

The polyhedron formed by the coordinated oxygen atoms about Yb(1) is a distorted capped trigonal prism

TABLE II

ATOMIC PARAMETERS OF $Yb(C_5H_7O_2)_3 \cdot 3H_2O$ WITH ESTIMATED STANDARD DEVIATIONS

	X	Y	Z	B, A
YB(1)	0.36456(10)	-0.24646(6)	-0.07908(14)	a
O(1-1)	0.4663(12)	-0.1970(8)	-0.2527(18)	3.6(4)
O(1-2)	0.2576(13)	-0.1802(8)	-0.1554(19)	3.5(4)
O(1-3)	0.2646(15)	-0.3141(10)	-0.3373(22)	5.1(5)
O(1-4)	0.2584(12)	-0.3469(9)	-0.0266(19)	4.0(4)
O(1-5)	0.4581(13)	-0.3338(9)	-0.1047(19)	3.8(4)
O(1-6)	0.5405(13)	-0.1752(9)	0.0928(20)	3.8(4)
O(1-7)	0.3409(14)	-0.1930(9)	0.1668(21)	4.9(4)
C(1-1)	0.1225(20)	-0.1242(14)	-0.2842(30)	3.8(6)
C(1-2)	0.1811(22)	-0.1883(15)	-0.2761(34)	3.7(6)
C(1-3)	0.1229(22)	-0.2531(16)	-0.4142(34)	6.0(8)
C(1-4)	0.1774(29)	-0.3101(19)	-0.4321(42)	8.4(9)
C(1-5)	0.1223(26)	-0.3816(18)	-0.6024(40)	8.2(1.0)
C(1-6)	0.1388(23)	-0.4689(15)	-0.0572(32)	5.6(7)
C(1-7)	0.2399(25)	-0.4196(17)	-0.0761(36)	5.9(8)
C(1-8)	0.3217(23)	-0.4496(15)	-0.1293(32)	3.8(7)
C(1-9)	0.4165(26)	-0.4112(18)	-0.1456(36)	6.0(8)
C(1-10)	0.5013(22)	-0.4444(15)	-0.2135(34)	6.0(8)
C(1-11)	0.7015(21)	-0.0987(14)	0.3024(32)	4.8(7)
C(1-12)	0.5194(22)	-0.1157(14)	0.3542(32)	4.0(7)
C(1-13)	0.5776(18)	-0.1344(12)	0.2448(28)	2.5(5)
C(1-14)	0.3997(22)	-0.1475(14)	0.3089(33)	3.3(7)
C(1-15)	0.3350(21)	-0.1235(14)	0.4316(31)	4.1(7)
YB(2)	0.23763(9)	0.20601(6)	0.25283(14)	b
O(2-1)	0.3334(11)	0.2414(7)	0.0542(16)	2.8(3)
O(2-2)	0.1150(13)	0.0958(10)	0.2470(20)	5.2(4)
O(2-3)	0.3197(13)	0.1167(9)	0.1728(19)	4.2(4)
O(2-4)	0.4018(13)	0.2524(9)	0.4323(20)	4.0(4)
O(2-5)	0.1976(15)	0.2342(10)	0.4961(23)	5.4(5)
O(2-6)	0.2676(13)	0.3331(9)	0.2877(19)	3.9(4)
O(2-7)	0.0926(14)	0.2118(9)	0.0832(20)	4.2(4)
C(2-1)	0.0004(26)	-0.0288(17)	0.2361(36)	7.0(9)
C(2-2)	0.1066(22)	0.0264(16)	0.2198(32)	4.5(7)
C(2-3)	0.1943(24)	-0.0034(15)	0.1763(33)	5.1(7)
C(2-4)	0.2918(21)	0.0424(15)	0.1541(30)	3.7(6)
C(2-5)	0.3751(21)	0.0055(14)	0.0976(32)	4.3(7)
C(2-6)	0.5633(23)	0.3430(15)	0.6533(33)	5.1(7)
C(2-7)	0.4394(26)	0.3003(17)	0.5856(40)	6.4(9)
C(2-8)	0.3665(23)	0.3187(15)	0.6808(32)	3.8(7)
C(2-9)	0.2496(26)	0.2838(17)	0.6359(40)	5.8(8)
C(2-10)	0.1800(25)	0.3046(17)	0.7548(38)	5.8(8)
C(2-11)	0.2395(23)	0.4555(16)	0.3375(35)	6.6(9)
C(2-12)	0.1917(29)	0.3643(19)	0.2545(42)	6.8(8)
C(2-13)	0.0850(25)	0.3389(17)	0.1367(36)	4.9(9)
C(2-14)	0.0374(25)	0.2581(18)	0.0468(37)	5.1(8)
C(2-15)	-0.0700(21)	0.2343(13)	-0.0763(30)	3.4(6)

a) β^{11}=0.00515(13), β^{22}=0.00214(6), β^{33}=0.01383(29)
β^{12}=0.00101(7), β^{13}=0.00125(15), β^{23}=-0.00013(10)

b) β^{11}=0.00533(13), β^{22}=0.00177(6), β^{33}=0.01575(29)
β^{12}=0.00115(7), β^{13}=0.00189(15), β^{23}=0.00051(10)

TABLE III

BOND LENGTHS AND ANGLES[a]

Lengths, A

Yb(1)-O(1-1)	2.313(14)	Yb(2)-O(2-1)	2.358(13)
Yb(1)-O(1-2)	2.173(13)	Yb(2)-O(2-2)	2.248(17)
Yb(1)-O(1-3)	2.214(17)	Yb(2)-O(2-3)	2.291(16)
Yb(1)-O(1-4)	2.204(16)	Yb(2)-O(2-4)	2.183(16)
Yb(1)-O(1-5)	2.295(16)	Yb(2)-O(2-5)	2.203(18)
Yb(1)-O(1-6)	2.326(16)	Yb(2)-O(2-6)	2.276(16)
Yb(1)-O(1-7)	2.232(16)	Yb(2)-O(2-7)	2.147(17)
O(1-2)-C(1-2)	1.21(3)	O(2-2)-C(2-2)	1.27(3)
O(1-3)-C(1-4)	1.28(3)	O(2-3)-C(2-4)	1.32(2)
O(1-4)-C(1-7)	1.30(3)	O(2-4)-C(2-7)	1.33(3)
O(1-5)-C(1-9)	1.36(3)	O(2-5)-C(2-9)	1.28(3)
O(1-6)-C(1-12)	1.27(2)	O(2-6)-C(2-12)	1.28(3)
O(1-7)-C(1-14)	1.28(3)	O(2-7)-C(2-14)	1.30(3)
C(1-2)-C(1-3)	1.42(3)	C(2-2)-C(2-3)	1.48(3)
C(1-4)-C(1-3)	1.44(4)	C(2-4)-C(2-3)	1.40(3)
C(1-7)-C(1-8)	1.44(3)	C(2-7)-C(2-8)	1.43(3)
C(1-9)-C(1-8)	1.30(3)	C(2-9)-C(2-8)	1.43(3)
C(1-12)-C(1-13)	1.37(3)	C(2-12)-C(2-13)	1.42(4)
C(1-14)-C(1-13)	1.45(3)	C(2-14)-C(2-13)	1.47(3)
C(1-2)-C(1-1)	1.59(3)	C(2-2)-C(2-1)	1.54(3)
C(1-4)-C(1-5)	1.65(4)	C(2-4)-C(2-5)	1.54(3)
C(1-7)-C(1-6)	1.45(3)	C(2-7)-C(2-6)	1.53(4)
C(1-9)-C(1-10)	1.56(4)	C(2-9)-C(2-10)	1.54(4)
C(1-12)-C(1-11)	1.51(3)	C(2-12)-C(2-11)	1.63(4)
C(1-14)-C(1-15)	1.53(3)	C(2-14)-C(2-15)	1.45(3)

Angles, degrees

O(1-2)-Yb(1)-O(1-3)	77.0(6)	O(2-2)-Yb(2)-O(2-3)	76.3(6)
O(1-4)-Yb(1)-O(1-5)	76.0(6)	O(2-4)-Yb(2)-O(2-5)	78.0(6)
O(1-6)-Yb(1)-O(1-7)	74.0(6)	O(2-6)-Yb(2)-O(2-7)	76.7(6)
Yb(1)-O(1-2)-C(1-2)	135.7(18)	Yb(2)-O(2-2)-C(2-2)	138.6(18)
Yb(1)-O(1-3)-C(1-4)	131.1(21)	Yb(2)-O(2-3)-C(2-4)	133.2(16)
Yb(1)-O(1-4)-C(1-7)	134.2(18)	Yb(2)-O(2-4)-C(2-7)	132.2(18)
Yb(1)-O(1-5)-C(1-9)	128.5(17)	Yb(2)-O(2-5)-C(2-9)	133.0(20)
Yb(1)-O(1-6)-C(1-12)	134.0(15)	Yb(2)-O(2-6)-C(2-12)	124.9(19)
Yb(1)-O(1-7)-C(1-14)	138.4(17)	Yb(2)-O(2-7)-C(2-14)	142.6(19)
O(1-2)-C(1-2)-C(1-3)	129.4(26)	O(2-2)-C(2-2)-C(2-3)	122.6(25)
O(1-3)-C(1-4)-C(1-3)	130.0(32)	O(2-3)-C(2-4)-C(2-3)	125.7(25)
O(1-4)-C(1-7)-C(1-8)	121.1(27)	O(2-4)-C(2-7)-C(2-8)	121.9(28)
O(1-5)-C(1-9)-C(1-8)	125.0(29)	O(2-5)-C(2-9)-C(2-8)	122.0(29)
O(1-6)-C(1-12)-C(1-13)	128.2(23)	O(2-6)-C(2-12)-C(2-13)	133.1(32)
O(1-7)-C(1-14)-C(1-13)	124.4(25)	O(2-7)-C(2-14)-C(2-13)	118.6(28)
O(1-2)-C(1-2)-C(1-1)	120.2(24)	O(2-2)-C(2-2)-C(2-1)	117.8(26)
O(1-3)-C(1-4)-C(1-5)	113.0(30)	O(2-3)-C(2-4)-C(2-5)	114.5(22)
O(1-4)-C(1-7)-C(1-6)	116.9(27)	O(2-4)-C(2-7)-C(2-6)	118.8(27)
O(1-5)-C(1-9)-C(1-10)	108.3(25)	O(2-5)-C(2-9)-C(2-10)	116.9(28)
O(1-6)-C(1-12)-C(1-11)	114.4(21)	O(2-6)-C(2-12)-C(2-11)	110.9(28)
O(1-7)-C(1-14)-C(1-15)	115.4(24)	O(2-7)-C(2-14)-C(2-15)	123.7(28)
C(1-1)-C(1-2)-C(1-3)	110.1(24)	C(2-1)-C(2-2)-C(2-3)	119.6(26)
C(1-5)-C(1-4)-C(1-3)	117.0(30)	C(2-5)-C(2-4)-C(2-3)	119.7(25)
C(1-6)-C(1-7)-C(1-8)	121.6(28)	C(2-6)-C(2-7)-C(2-8)	119.0(28)
C(1-10)-C(1-9)-C(1-8)	126.7(30)	C(2-10)-C(2-9)-C(2-8)	121.2(29)
C(1-11)-C(1-12)-C(1-13)	117.2(23)	C(2-11)-C(2-12)-C(2-13)	114.6(30)
C(1-15)-C(1-14)-C(1-13)	120.1(25)	C(2-15)-C(2-14)-C(2-13)	117.6(29)
C(1-2)-C(1-3)-C(1-4)	114.5(28)	C(2-2)-C(2-3)-C(2-4)	123.6(26)
C(1-7)-C(1-8)-C(1-9)	127.2(29)	C(2-7)-C(2-8)-C(2-9)	125.7(28)
C(1-12)-C(1-13)-C(1-14)	120.8(25)	C(2-12)-C(2-13)-C(2-14)	118.8(29)

[a] Chemically equivalent dimensions are grouped together.

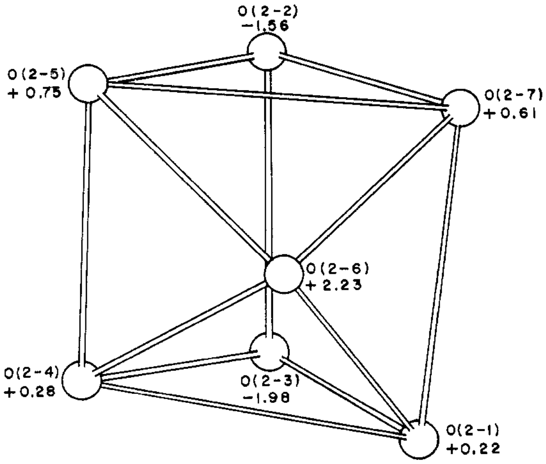

Figure 4.—Coordination polyhedron formed by the seven oxygen atoms bonded to Yb(2). The distance of each atom from the central plane is given. The view is along a vector 30° from Yb(2)–O(2-3) in the plane of Yb(2)–O(2-3)–O(2-2).

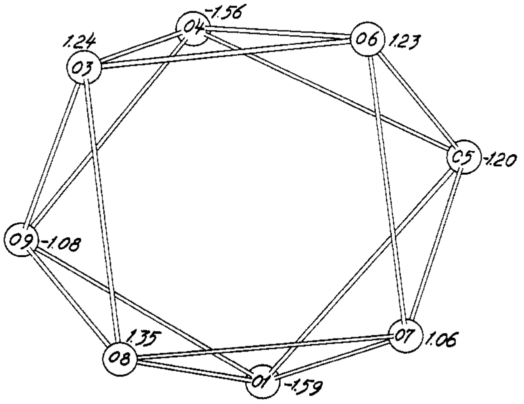

Figure 5.—Coordination polyhedron in $Y(C_5H_7O_2)_3 \cdot 3H_2O$ formed by the eight oxygen atoms bonded to the yttrium ion. The distance of each atom from the central plane is given.

with O(1-3) capping the lateral face O(1-1)–O(1-2)–O(1-4)–O(1-5). Distances related by the ideal C_{2v} symmetry of this polyhedron are grouped together in Table IV. A capped trigonal prism was observed in the structure of the NbF_7^{2-} ion.[17] In the present case, however, the distortions resulting from chemically different ligands make it difficult to distinguish this polyhedron from the tetragonal base–trigonal base geometry reported for $(C_6H_5)_4C_4Fe(CO)_3$.[18] Descrip-

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(17) J. L. Hoard, *J. Am. Chem. Soc.*, **61**, 1252 (1939).

(18) R. P. Dodge and V. Schomaker, *Nature*, **186**, 798 (1960).

TABLE IV
DIMENSIONS OF COORDINATION POLYHEDRA

DISTANCES, A

O(1-2)-O(1-4)	3.50	O(2-7)-O(2-5)	3.33
O(1-5)-O(1-1)	3.04	O(2-4)-O(2-1)	3.04
O(1-7)-O(1-6)	2.74	O(2-2)-O(2-3)	2.80
O(1-4)-O(1-5)	2.77	O(2-5)-O(2-4)	2.76
O(1-2)-O(1-1)	3.07	O(2-7)-O(2-1)	3.10
O(1-4)-O(1-3)	2.78	O(2-5)-O(2-6)	2.87
O(1-2)-O(1-3)	2.73	O(2-7)-O(2-6)	2.75
O(1-3)-O(1-5)	2.99	O(2-6)-O(2-4)	2.82
O(1-3)-O(1-1)	2.81	O(2-6)-O(2-1)	2.78
O(1-2)-O(1-7)	2.75	O(2-7)-O(2-2)	2.82
O(1-4)-O(1-7)	2.85	O(2-5)-O(2-2)	2.81
O(1-1)-O(1-6)	2.75	O(2-1)-O(2-3)	2.69
O(1-5)-O(1-6)	2.93	O(2-4)-O(2-3)	2.82
O(1-1)-O(1-7)	4.15	O(2-1)-O(2-2)	4.19
O(1-2)-O(1-6)	3.79	O(2-7)-O(2-3)	3.85
O(1-7)-O(1-5)	3.98	O(2-2)-O(2-4)	3.90
O(1-6)-O(1-4)	4.00	O(2-3)-O(2.5)	4.02

ANGLES, DEGREES

O(1-2)-O(1-4)-O(1-7)	50.1	O(2-7)-O(2-5)-O(2-2)	54.0
O(1-4)-O(1-7)-O(1-2)	77.3	O(2-5)-O(2-2)-O(2-7)	72.4
O(1-7)-O(1-2)-O(1-4)	52.6	O(2-2)-O(2-7)-O(2-5)	53.6
O(1-2)-O(1-3)-O(1-4)	78.8	O(2-7)-O(2-6)-O(2-5)	72.5
O(1-3)-O(1-4)-O(1-2)	50.0	O(2-6)-O(2-5)-O(2-7)	52.0
O(1-4)-O(1-2)-O(1-3)	51.2	O(2-5)-O(2-7)-O(2-6)	55.5
O(1-1)-O(1-3)-O(1-5)	63.1	O(2-1)-O(2-6)-O(2-4)	65.6
O(1-3)-O(1-5)-O(1-1)	55.5	O(2-6)-O(2-4)-O(2-1)	56.6
O(1-5)-O(1-1)-O(1-3)	61.4	O(2-4)-O(2-1)-O(2-6)	57.8
O(1-3)-O(1-4)-O(1-5)	65.2	O(2-6)-O(2-5)-O(2-4)	60.1
O(1-4)-O(1-5)-O(1-3)	57.6	O(2-5)-O(2-4)-O(2-6)	61.8
O(1-5)-O(1-3)-O(1-4)	57.2	O(2-4)-O(2-6)-O(2-5)	58.1
O(1-1)-O(1-2)-O(1-3)	57.5	O(2-1)-O(2-7)-O(2-6)	56.4
O(1-2)-O(1-3)-O(1-1)	67.3	O(2-7)-O(2-6)-O(2-1)	68.3
O(1-3)-O(1-1)-O(1-2)	55.2	O(2-6)-O(2-1)-O(2-7)	55.3
O(1-1)-O(1-5)-O(1-6)	54.9	O(2-1)-O(2-4)-O(2-3)	54.4
O(1-5)-O(1-6)-O(1-1)	64.5	O(2-4)-O(2-3)-O(2-1)	67.0
O(1-6)-O(1-1)-O(1-5)	60.6	O(2-3)-O(2-1)-O(2-4)	58.6
O(1-1)-O(1-2)-O(1-7)	90.8	O(2-1)-O(2-7)-O(2-2)	90.0
O(1-2)-O(1-7)-O(1-6)	87.3	O(2-7)-O(2-2)-O(2-3)	86.4
O(1-1)-O(1-6)-O(1-7)	98.1	O(2-1)-O(2-3)-O(2-2)	99.6
O(1-2)-O(1-1)-O(1-6)	81.1	O(2-7)-O(2-1)-O(2-3)	83.0
O(1-4)-O(1-7)-O(1-6)	91.4	O(2-5)-O(2-2)-O(2-3)	91.5
O(1-5)-O(1-4)-O(1-7)	90.4	O(2-4)-O(2-5)-O(2-2)	88.7
O(1-4)-O(1-5)-O(1-6)	89.1	O(2-5)-O(2-4)-O(2-3)	92.1
O(1-5)-O(1-6)-O(1-7)	89.1	O(2-4)-O(2-3)-O(2-2)	87.7

STANDARD DEVIATIONS OF DISTANCES = 0.02 A
STANDARD DEVIATION OF ANGLES = 0.4 to 0.7 DEGREES

tion is also possible in terms of the capped octahedron which has been found in the chelate structures tris(diphenylpropanedionato)aquoholmium[19] and tris(1-phenyl-1,3-butanedionato)aquoyttrium(III).[20] The capping ligand in this case would be the carbonyl oxygen atom O(1-7) rather than a water molecule, and the deviations from a regular octahedron would be large.[21]

The polyhedron about Yb(2) may also be described as a capped trigonal prism with O(2-6) as the capping ligand. Description is also possible as a tetragonal base–trigonal base figure with bases O(2-2)–O(2-3)–O(2-4)–O(2-5) and O(2-1)–O(2-6)–O(2-7) or as a tetragonal base–trigonal base figure with bases O(2-1)–O(2-3)–O(2-2)–O(2-7) and O(2-4)–O(2-5)–O(2-6). Corresponding dimensions of the two polyhedra, interpreted as capped trigonal prisms, are adjacent in Table IV.

In $Y(C_5H_7O_2)_3 \cdot 3H_2O$[6] the polyhedron formed by the eight coordinated oxygen atoms is a distorted square antiprism (Figure 5). The coordination polyhedron about Yb(1) or Yb(2) can be derived from this square antiprism by removing the coordinated water molecule O(1) and shifting the carbonyl oxygen atom O(4) to this vertex. The line passing through O(5)–O(9) would constitute an edge of the new polyhedron, and the O(3)–O(6)–O(7)–O(8) quadrilateral would correspond to the O(1-4)–O(1-5)–O(1-6)–O(1-7) quadrilateral in the monohydrated ytterbium chelate.

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(19) A. Zalkin and D. H. Templeton, American Crystallographic Association Meeting, Minneapolis, Minn., Aug 1967, paper T7.

(20) F. A. Cotton and P. Legzdins, *Inorg. Chem.*, **7**, 1777 (1968).

(21) See E. L. Muetterties and C. M. Wright, *Quart. Rev.* (London), **21**, 109 (1967), for a summary of the stereochemistry of higher coordination.