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The Crystal Structure of NN'-ethylenebis-(acetylacetoneiminato)vinylaquocobalt(III)

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The crystal and molecular structure of NN'-ethylenebis-(acetylacetoneiminato)vinylaquocobalt(III) has been determined using three-dimensional X-ray diffraction data. There are four molecules in the monoclinic unit cell, space group $P2_1/n$, with dimensions, a = 9.19 Å, b = 14.32 Å, c = 11.95 Å, β = 99.1°. Final refinement was by block-diagonal anisotropic least-squares adjustment to an R of 0.078. The coordination around the cobalt atom is that of a distorted octahedron. The tetradentate ligand occupies the equatorial coordination sites. A water molecule and a σ-bonded vinyl group in the axial positions complete the coordination polyhedron. The bond lengths are 1.92 Å (mean) for Co–O, 1.89 Å (mean) for Co–N, 1.89 Å for Co–C, and 2.22 Å for Co–OH_2. Intermolecular hydrogen bonds O–H.....O, involving the oxygen atoms of the tetradentate ligand and the water molecule of two complex molecules related by a symmetry centre are found.

Introduction

In the previous paper[1] the crystal structure determination of the lattice compound between NN'-ethylenebis-(acetylacetoneiminato)cobalt(II), Co(BAE), and benzene, carried out as a part of a research program on the structure of some stable organometallic derivatives of cobalt(III) chelates, has been described.

We report here on the crystal structure of NN'-ethylenebis-(acetylacetoneiminato)vinylaquocobalt(III) ($C_2H_3Co(BAE)H_2O$).

Experimental Section

Single red monoclinic crystals elongated along [001], prepared as previously described,[2] were kindly supplied by Professor G. Costa and Dr. G. Mestroni of this Institute.

The cell dimensions, determined from precession photographs, taken with MoK_α radiation, are: $a = 9.19 \pm 0.02$ Å, $b = 14.32 \pm 0.02$ Å, $c = 11.95 \pm 0.02$ Å, $\beta = 99.1 \pm 0.3°$.

The calculated density, assuming four formula units, $C_2H_3Co(BAE)H_2O$, per unit cell, is 1.40 g.cm^{-3} in good agreement with the value of 1.42 g.cm^{-3} of the density measured by flotation method.

Systematic absences, h0l with h+l odd and 0k0 with k odd, indicated the space group $P2_1/n$.

Intensity data were collected by the equi-inclination Weissenberg method using MoK_α radiation. Levels h0l through h15l and hk0 through hk7 were recorded by the multiple film technique.

The intensities of 1513 reflections were measured by visual comparison with a standard scale and were placed in a common scale by cross-correlation terms. No correction for absorption was made. Lorentz and polarization factors and the spot shape correction for non-zero levels were applied.

All calculations were carried out on a IBM 7044 computer with programs written by A. Domenicano *et al.*[3,4]

The atomic scattering factors used were those of Hanson *et al.*[5] for oxygen, carbon and hydrogen, that of Berghuis *et al.*[6] for nitrogen and that, listed in the International Tables for X-Ray Crystallography,[7] for cobalt.

Structure Determination

Approximate position of the cobalt atom was readily determined from peak locations on a three-dimensional Patterson map.

A cobalt-phased three-dimensional electron density map showed clearly all the other non-hydrogen atoms. After a cycle of Fourier refinement the R-value was 0.17 using an overall isotropic temperature factor of 1.5 Å^2. The atomic parameters were then refined by isotropic block-diagonal least-squares method. The R-value fell to 0.114 after five cycles. Three more cycles of refinement of all atomic coordinates and anisotropic temperature factors for each atom lowered the R-value to 0.092. At this stage a three-dimensional difference Fourier synthesis was calculated. Estimated

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(1) S. Brückner, M. Calligaris, G. Nardin, and L. Randaccio, *Inorg. Chim. Acta, 2,* 386 (1968).
(2) G. Costa and G. Mestroni, *J. Organometal. Chem., 11,* 325 (1968).
(3) V. Albano, A. Domenicano, and A. Vaciago, *Gazz. Chim. Ital.,* 96, 922 (1966).
(4) A. Domenicano and A. Vaciago, private communication.
(5) H. P. Hanson, F. Herman, J. D. Lea, and S. Skillman, *Acta Cryst., 17,* 1040 (1964).
(6) J. Berghuis, I. J. M. Haanappell, M. Potters, B. O. Loopstra, C. H. Gillavry, and A. L. Veenedaal, *Acta Cryst., 8,* 478 (1955).
(7) «International Tables for X-ray Crystallography», vol. III, Kynoch Press, Birmingham (1962).

Table I. Fractional atomic coordinates and their standard deviations in parentheses. All value are multiplied by 10^4.

Atom	x	y	z
Co	281 (1)	33 (1)	2119 (1)
N(1)	311 (9)	1183 (5)	2895 (7)
N(2)	—1290 (8)	— 311 (5)	2884 (7)
O(1)	1784 (7)	369 (5)	1254 (5)
O(2)	129 (7)	—1110 (5)	1252 (6)
O(3)	—1304 (8)	690 (5)	749 (6)
C(1)	3671 (12)	1233 (9)	600 (11)
C(2)	2478 (11)	1164 (8)	1341 (9)
C(3)	2226 (11)	1878 (7)	2032 (9)
C(4)	1212 (11)	1888 (7)	2817 (9)
C(5)	1163 (14)	2754 (8)	3541 (11)
C(6)	— 630 (12)	1170 (7)	3788 (9)
C(7)	—1907 (11)	508 (7)	3377 (8)
C(8)	—3051 (13)	—1325 (8)	3667 (10)
C(9)	—1857 (10)	—1135 (7)	2960 (9)
C(10	—1369 (12)	—1943 (7)	2376 (9)
C(11)	— 503 (10)	—1861 (6)	1528 (8)
C(12)	— 309 (12)	—2706 (8)	813 (10)
C(13)	1635 (11)	— 529 (7)	3279 (9)
C(14)	3003 (13)	— 248 (8)	3671 (11)

Table II. Final anisotropic temperature factors and their standard deviations in parentheses. The temperature factor is of the form $\exp -(B_{11}h^2+B_{12}hk+B_{13}hl+B_{22}k^2+B_{23}kl+B_{33}l^2)$. All values are multiplied by 10^4

Atom	B_{11}	B_{12}	B_{13}	B_{22}	B_{23}	B_{33}
Co	51 (1)	– 6 (2)	42 (1)	15 (0)	– 3 (2)	38 (1)
N(1)	65 (9)	9 (10)	21 (12)	24 (3)	– 9 (8)	40 (6)
N(2)	67 (9)	–18 (9)	37 (11)	19 (3)	– 1 (7)	45 (5)
O(1)	75 (7)	–10 (9)	80 (9)	37 (3)	9 (7)	56 (5)
O(2)	60 (7)	–12 (8)	55 (10)	29 (3)	–18 (7)	58 (5)
O(3)	99 (9)	3 (11)	57 (11)	44 (4)	– 9 (8)	52 (5)
C(1)	75 (13)	–62 (16)	79 (20)	63 (7)	–24 (15)	102 (11)
C(2)	70 (12)	–35 (14)	25 (16)	40 (5)	12 (11)	54 (7)
C(3)	77 (12)	–44 (13)	34 (16)	37 (5)	9 (11)	56 (8)
C(4)	72 (12)	8 (14)	2 (16)	32 (5)	– 5 (10)	50 (7)
C(5)	120 (16)	– 4 (16)	44 (21)	38 (6)	–24 (13)	81 (10)
C(6)	90 (12)	13 (13)	64 (15)	32 (5)	–16 (10)	58 (7)
C(7)	114 (12)	22 (12)	91 (13)	23 (4)	–25 (9)	61 (7)
C(8)	127 (14)	–42 (15)	118 (16)	44 (6)	– 5 (12)	75 (8)
C(9)	56 (11)	–23 (12)	45 (15)	35 (5)	3 (11)	59 (8)
C(10)	96 (13)	– 7 (14)	49 (17)	28 (5)	–10 (10)	64 (8)
C(11)	66 (11)	0 (11)	24 (14)	18 (4)	1 (9)	51 (7)
C(12)	92 (13)	–23 (14)	43 (19)	34 (5)	–30 (12)	80 (10)
C(13)	94 (12)	8 (13)	66 (15)	25 (5)	5 (10)	59 (7)
C(14)	121 (15)	–16 (15)	32 (20)	35 (6)	14 (12)	79 (10)

positions for the hydrogen atoms all occurred in regions of positive electron density. Therefore the hydrogen atoms were included at the calculated positions and a final least-squares refinement lowered the R-value to 0.078. The contribution of the hydrogen atoms was held constant, with an overall isotropic temperature factor of 5 Å^2. The reflections 110, 002, 112 were omitted from refinement as they most probably suffer from extinction. The weighting scheme used was:

$$w = 1/(7.10 + 1.00|F_o| + 0.01|F_o|^2)$$

The final parameters of all the non-hydrogen atoms are listed in Table I and Table II together with their estimated standard deviations. The coordinates of the hydrogen atoms are listed in Table III. Observed and calculated structure factors are listed in Table IV.

Table III. Fractional coordinates of hydrogen atoms (multiplied by 10^3)

Atom	x	y	z
H(1C1)	422	190	77
H(2C1)	321	118	–26
H(3C1)	446	68	85
H(1C3)	286	251	198
H(1C5)	198	324	338
H(2C5)	137	256	443
H(3C5)	8	306	336
H(1C6)	0	90	457
H(2C6)	–102	185	394
H(1C7)	–271	85	276
H(2C7)	–245	29	408
H(1C8)	–332	–205	364
H(2C8)	–402	– 92	337
H(3C8)	–265	–113	454
H(1C10)	–169	–262	263
H(1C12)	– 94	–328	106
H(2C12)	82	–289	88
H(3C12)	– 72	–253	–8
H(1C13)	126	–114	367
H(1C14)	367	– 63	433
H(2C14)	345	36	331
H(1O3)	–180	19	24
H(2O3)	– 75	108	26

Results and Discussion

Bond lengths and angles are given in Table V. The numbering scheme for the atoms is shown in Figure 1.

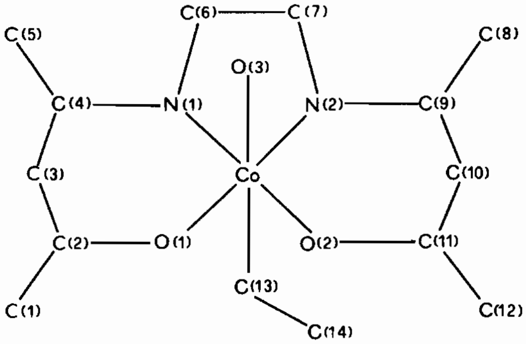

Figure 1. Numbering scheme for the atoms of the complex molecule.

The coordination about the cobalt atom is that of a distorted octahedron with coplanar atoms Co, O(1), O(2), N(1), and N(2) lying in the equatorial plane, and the water molecule and the vinyl group occupying the axial positions. The vinyl group is σ-bonded to the cobalt atom *via* one carbon atom. The Co–C(13) bond length is found to be 1.89 Å. The C(13)–C(14) bond length of 1.33 Å and the Co–C(13)–C(14) bond angle of 127.2° may be indicative that the metal-carbon bond is single. On the other hand the shortening of the Co–C(13) distance with respect to the sum of the covalent radii of octahedral cobalt(III) (1.28 Å)[8] and of the sp^2-hybridised carbon (0.74 Å) is consistent with the view that this bond has some

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(8) R. Mason, and D. R. Russell, *Chem. Comm.*, 182 (1965).

Table IV. Observed and calculated structure factors (x10)

H	K	FO	|FC|
******L=		0******	
0	2	1162	1270
0	4	492	457
0	6	555	555
0	8	644	671
0	10	667	678
0	16	398	439
0	18	212	256
1	1	1559	2191
1	2	798	738
1	3	713	719
1	4	621	601
1	5	497	486
1	6	331	298
1	7	696	678
1	8	99	79
1	9	506	519
1	10	189	171
1	11	600	605
1	12	343	333
1	15	327	351
1	17	274	319
1	19	188	192
1	21	165	151
2	0	590	554
2	1	482	438
2	2	280	257
2	3	842	791
2	4	547	518
2	5	163	150
2	6	505	465
2	7	462	436
2	8	780	773
2	10	662	683
2	11	292	310
2	12	444	460
2	13	214	214
2	14	301	309
2	16	217	276
2	18	223	254
3	1	452	423
3	2	227	217
3	3	214	186
3	5	168	150
3	6	333	311
3	7	982	957
3	8	282	279
3	9	864	867
3	11	434	458
3	12	215	180
3	13	324	331
3	15	248	249
3	17	262	232
3	19	107	145
4	0	329	315
4	1	123	91
4	2	440	436
4	3	121	133
4	4	192	153
4	6	432	443
4	8	713	731
4	10	455	464
4	11	154	147
4	12	275	293
4	14	178	158
4	16	175	201
4	18	243	220
5	1	579	586
5	3	388	343
5	4	97	84
5	5	178	149
5	7	293	296
5	9	347	372
5	10	184	154
5	11	179	175
5	15	141	116
5	17	201	209
5	19	181	182
5	21	118	87
6	0	632	630
6	2	526	519
6	3	165	141
6	4	278	265
6	5	198	145
6	8	215	209
6	10	122	89
7	1	320	314
7	3	272	267
7	5	168	123
9	8	96	114
9	12	105	144
11	1	124	77
******L=		1******	
0	1	422	384
0	4	201	154
0	9	193	124
0	11	246	232
1	0	217	193
-1	0	699	836
1	1	215	179
-1	-1	126	111
1	2	168	158
-1	-2	318	278
1	3	450	408
-1	-3	73	70
-1	-4	734	745
1	5	171	140
1	6	185	133
-1	-6	405	342
1	7	241	199
-1	-7	231	176
-1	-8	172	127
1	9	253	282
-1	-10	259	243
1	11	228	192
-1	-12	239	226
2	1	400	327
-2	-1	370	318
2	2	101	89
-2	-2	163	132
-2	-3	576	496
2	4	87	50
-2	-4	308	303
-2	-5	329	299
-2	-6	374	300
2	7	140	119
-2	-7	560	504
2	8	141	142
-2	-9	241	194
2	10	313	307
-2	-10	219	200
-2	-11	315	320
-2	-13	223	201
2	14	139	90
-2	-14	170	167
-2	-15	247	224
3	0	126	108
-3	0	514	421
3	1	177	137
-3	-1	267	209
3	2	602	506
-3	-2	166	143
-3	-3	328	295
3	4	166	157
-3	-4	379	324
3	5	362	285
-3	-5	168	139
3	6	168	151
-3	-6	271	230
3	7	207	153
3	8	194	185
-3	-8	674	639
3	9	155	140
-3	-9	179	119
-3	-10	394	353
3	11	142	139
-3	-11	165	130
3	12	140	132
-3	-12	334	256
3	14	231	203
-3	-14	295	262
-3	-16	237	186
-3	-18	305	273
4	1	500	423
-4	-1	651	560
-4	-2	279	210
4	3	483	436
-4	-3	644	589
4	4	125	79
-4	-4	164	121
4	5	166	143
-4	-5	389	339
4	6	134	103
-4	-6	346	318
4	7	223	199
-4	-7	653	632
-4	-8	157	127
4	9	338	328
-4	-9	582	542
4	10	181	179
-4	-10	295	258
-4	-11	466	422
4	12	193	170
4	13	305	275
-4	-13	212	171
5	0	276	212
-5	0	1147	1054
5	1	163	142
-5	-1	252	212
5	2	514	471
-5	-2	691	622
-5	-3	233	201
5	4	185	173
-5	-4	427	379
5	5	177	164
5	6	291	247
-5	-6	570	541
5	7	296	286
-5	-7	360	361
5	8	228	224
-5	-8	691	696
5	9	161	131
-5	-9	266	267
5	10	303	261
-5	-10	520	506
5	11	156	109
5	12	254	227
-5	-12	245	186
5	14	211	183
-5	-14	202	168
5	16	188	175
-5	-16	160	187
6	1	527	490
-6	-1	754	763
-6	-2	413	394
6	3	329	306
-6	-3	554	512
6	4	151	119
6	5	407	376
-6	-5	477	432
6	6	236	196
-6	-6	170	168
6	7	279	263
-6	-7	479	467
6	8	200	189
6	9	362	350
-6	-9	474	482
-6	-11	263	231
6	13	251	201
-6	-13	281	243
-6	-14	199	175
-6	-15	221	202
7	0	343	336
-7	0	432	442
7	2	547	544
-7	-2	789	784
7	3	157	143
7	4	476	464
-7	-4	511	468
7	5	246	226
-7	-5	266	224
7	6	439	420
-7	-6	340	277
7	7	131	143
-7	-7	244	219
7	8	301	300
-7	-8	363	345
7	10	143	151
-7	-10	287	267
7	12	152	163
-7	-12	285	245
-7	-14	247	214
8	1	255	268
-8	-1	579	635
8	3	479	481
-8	-3	415	385
8	5	369	367
-8	-6	212	169
8	7	269	268
-8	-7	323	337
8	9	214	223
-8	-9	433	459
8	11	200	170
8	13	212	204
-8	-13	162	192
9	0	336	357
-9	0	399	434
9	2	223	244
-9	-2	339	338
9	4	166	147
9	6	224	223
-9	-6	204	187
9	8	294	322
-9	-8	384	405
9	10	246	239
-9	-10	289	266
9	12	167	148
10	1	259	280
-10	-1	256	222
10	2	214	153
10	5	238	186
10	7	261	260
-10	-7	242	226
10	9	271	231
-10	-9	287	290
10	11	199	217
-10	-11	241	213
11	0	246	219
-11	0	243	237
-11	-2	187	163
11	4	231	189
-11	-6	190	195
-11	-8	196	235
12	1	169	176
******L=		2******	
0	0	1163	1899
0	1	272	293
0	2	587	719
0	3	746	891
0	4	670	760
0	5	318	336
0	6	806	966
0	7	369	383
0	8	345	380
0	9	262	301
0	10	548	609
0	12	245	185
0	16	377	322
1	1	1381	1866
-1	-1	679	708
1	2	838	896
-1	-2	120	115
1	3	100	108
-1	-3	668	748
1	4	356	378
1	5	708	755
-1	-5	832	941
1	6	426	411
-1	-6	757	797
1	7	695	804
-1	-7	408	420
1	8	110	130
-1	-8	106	101
1	9	697	806
-1	-9	309	350
1	11	231	239
-1	-11	461	535
1	12	356	381
-1	-13	236	257
1	14	206	210
-1	-14	156	163
1	15	194	232
-1	-15	280	302
-1	-16	179	116
1	17	345	297
-1	-17	187	207
2	0	285	280
-2	0	615	618
2	1	1390	1560
-2	-1	356	341
2	2	1308	1456
-2	-2	126	111
2	3	613	612
-2	-3	294	256
2	4	747	760
-2	-4	218	236
2	5	246	250
-2	-5	128	102
2	6	835	887
-2	-6	376	369
2	7	119	82
-2	-7	449	405
2	8	675	789
-2	-8	377	399
-2	-9	191	155
2	10	449	477
-2	-10	396	392
2	11	436	463
2	12	309	305
-2	-12	345	366
2	14	212	214
-2	-14	360	370
2	15	214	185
-2	-16	317	273
-2	-18	196	155
3	1	377	380
-3	-1	365	365
3	2	593	608
-3	-2	270	242
3	3	879	946
-3	-3	423	357
3	4	398	364
-3	-4	300	216
3	5	526	554
-3	-5	230	197
3	6	225	178
-3	-6	250	194
3	7	581	644
-3	-7	339	315
-3	-8	158	156
3	9	651	730
-3	-9	223	171
3	11	279	299
-3	-11	317	305
3	12	174	128
3	13	510	545
-3	-13	275	256
3	15	205	177
-3	-15	260	220
4	0	296	300
-4	0	640	606
-4	-1	227	176
4	2	574	618
-4	-2	519	477
4	3	477	479
-4	-3	390	316
-4	-4	277	328
4	5	218	170
-4	-5	110	71
4	6	352	346
-4	-6	265	211
-4	-7	196	177
4	8	645	709
-4	-8	187	150
4	10	388	399
-4	-10	175	141
4	12	388	392
-4	-12	172	148
4	14	374	388
4	16	290	293
4	18	263	255
5	1	638	688
-5	-1	152	119
5	2	166	161
5	3	431	415
-5	-3	202	165
5	4	133	99
-5	-4	166	128
5	5	190	180
-5	-5	207	164
5	6	240	181
5	7	338	316
-5	-7	163	134
5	9	409	447
5	10	148	121
5	11	292	270
5	13	316	296
5	15	259	238
6	0	633	748
-6	0	192	192
6	2	555	613
6	4	348	331
6	5	247	225
6	6	282	241
6	7	276	246
6	8	307	320
-6	-9	155	151
6	10	304	282
7	1	350	408
7	3	332	329
-7	-4	145	118
7	5	278	267
7	6	274	267
7	7	245	263
7	9	238	229
-7	-10	179	182
-8	-2	244	233
-8	-3	165	136
8	4	263	249
8	6	260	247
8	8	167	153
-8	-8	174	210
-9	-3	125	168
9	5	179	177
-9	-6	181	160
-9	-9	207	222
-10	-2	159	169
-10	-6	219	241
-11	-5	241	269
******L=		3******	
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1	6	359	381
-1	-6	176	155
1	8	216	214
-1	-8	276	307
1	10	248	295
1	12	256	231
1	14	243	235
-1	-14	168	178
2	1	194	208
-2	-1	284	289
2	2	180	158
2	3	291	286
-2	-3	376	407
2	5	402	414
-2	-6	132	121
2	7	276	304
-2	-7	310	307
2	9	350	343
-2	-9	204	215
2	11	255	279
2	13	277	253
-2	-13	266	228
3	0	267	267
3	2	330	342
-3	-2	153	136
3	3	179	142
-3	-3	249	235
3	4	229	218
-3	-4	274	262
3	6	317	308
3	8	296	325
-3	-8	165	149
-3	-9	207	215
3	10	318	342
-3	-10	153	145
-3	-11	149	137
3	12	233	220
-3	-12	232	238
-3	-14	132	152
4	1	383	426
-4	-1	116	117
4	3	199	196
-4	-3	194	180
-4	-4	151	150
4	5	195	224
-4	-5	180	171
4	7	216	245
4	9	302	286
-4	-10	185	126
5	0	416	416
-5	0	176	161
5	2	332	337
5	4	276	264
5	6	279	253
6	1	294	292
6	3	219	225
6	5	250	210
6	6	178	127
-8	-3	217	216
-8	-5	183	192
-9	-2	210	244
-9	-4	273	269
-9	-6	151	198
-10	-5	233	238
******L=		10******	
0	0	270	267
0	2	281	311
0	4	254	225
0	6	242	232
0	7	144	133
0	8	243	259
0	9	191	177
0	10	246	235
0	12	152	170
1	1	160	147
-1	-1	496	577
-1	-2	200	224
1	3	178	166
-1	-3	347	374
1	5	257	207
-1	-5	129	126
1	6	180	174
1	7	232	221
-1	-7	287	322
1	9	232	229
-1	-9	313	312
1	11	158	162
-2	0	597	610
-2	-1	145	142
-2	-2	587	664
-2	-3	343	355
-2	-4	321	355
-2	-6	207	188
2	8	203	170
-2	-8	347	373
-2	-10	188	144
-3	-1	360	385
-3	-3	530	560
-3	-4	117	125
-3	-5	273	274
-3	-6	126	130
-3	-7	310	280
-3	-9	241	206
-3	-10	239	209
-3	-11	248	232
-3	-13	219	244
-4	0	401	432
-4	-1	212	198
-4	-2	166	177
-4	-4	257	251
-4	-6	286	271
-4	-8	336	356
-4	-10	378	348
-4	-12	248	250
-4	-14	258	247
-5	-1	282	311
-5	-3	140	121
-5	-5	278	269
-5	-6	176	178
-5	-7	423	417
-5	-9	372	408
-5	-11	358	394
-6	0	341	363
-6	-2	251	221
-6	-4	364	344
-6	-6	300	323
-6	-8	311	352
-6	-10	341	363
-6	-12	185	205
-7	-1	355	356
-7	-3	319	310
-7	-5	285	283
-7	-7	307	292
-7	-9	216	191
-8	0	360	349
-8	-2	309	322
-8	-4	312	311
-8	-6	235	233
-9	-1	211	242
-9	-3	219	226
-9	-5	255	209
******L=		11******	
0	1	167	181
0	3	140	125
1	0	250	246
1	2	245	213
-1	-2	181	165
1	4	199	198
1	6	233	210
-1	-8	180	180
2	1	245	239
2	3	145	118
2	5	282	274
2	9	157	140
3	0	181	185
3	4	161	149
3	6	200	174
3	8	163	153
3	10	196	202
3	12	225	182
4	1	232	243
4	9	236	200
5	0	359	342
5	2	210	199
5	6	228	182
-5	-6	170	141
6	1	186	195
-6	-1	153	151
-6	-3	200	172
6	5	216	175
-6	-5	196	197
-6	-7	246	216
-7	0	340	316
-7	-2	250	244
-7	-4	276	274
-7	-6	222	204
-7	-8	152	174
-8	-3	330	289
-8	-5	232	216
-9	0	346	333
-10	-1	213	282
******L=		12******	
0	0	441	458
0	2	315	312
0	3	148	108
0	6	300	284
0	8	353	374
0	10	325	268
1	1	296	309
-1	-1	358	382
-1	-2	214	211
1	3	150	151
-1	-3	247	245
1	4	174	137
1	5	220	204
-1	-5	190	164
-1	-7	307	326
1	9	243	254
-1	-9	395	363
1	11	213	192
2	0	283	268
-2	-2	415	427
-2	-3	147	138
-2	-4	282	248
-2	-6	241	206
2	8	167	153
-2	-8	284	285
3	1	236	217
-3	-1	338	333
-3	-3	312	290
-3	-5	205	163
-3	-7	266	229
-3	-9	277	271
-4	0	354	344
-4	-2	258	272
-4	-6	201	178
-4	-8	254	265
-4	-10	278	259
-5	-1	251	257
-5	-9	262	265
-5	-11	235	207
-6	0	242	258
-6	-2	263	235
-6	-4	196	194
-6	-6	182	170
-6	-8	230	209
-7	-1	147	170
-7	-3	231	200
-7	-7	196	158
******L=		13******	
3	4	145	111
-4	-1	247	224
-5	0	367	352
-5	-2	290	309
-5	-8	191	164
-6	-1	332	360
-6	-3	247	236
-7	-2	271	273
-7	-4	223	220
-7	-6	178	185
-7	-8	231	225
-8	-1	158	199
-9	0	326	317
-9	-8	229	280
******L=		14******	
0	0	365	364
0	2	227	182
0	4	204	156
0	6	204	180
1	1	304	289
1	5	198	162
-1	-5	210	182
2	0	269	249
-2	-6	167	143
-3	-1	148	143
-3	-7	176	168
******L=		15******	
-4	-1	248	236
-5	0	395	335
-5	-2	314	296
-6	-1	243	241
-6	-3	297	261
-7	-2	223	219
******L=		16******	
0	0	139	106

Table V. Bond lengths (Å) and angles (°). Their standard deviations are given in parentheses

Co–N(1)	1.888 (.008) Å	N(1)–Co–N(2)	86.7 (.4)°	Co–O(1)–C(2)	124.3 (.7)
Co–N(2)	1.892 (.008)	N(1)–Co–O(1)	95.2 (.3)	Co–O(2)–C(11)	124.6 (.6)
Co–O(1)	1.913 (.007)	N(2)–Co–O(2)	92.4 (.3)	O(1)–C(2)–C(1)	113.6 (1.)
Co–O(2)	1.930 (.007)	O(1)–Co–O(2)	85.4 (.3)	O(1)–C(2)–C(3)	125.4 (1.)
Co–O(3)	2.221 (.007)	N(1)–Co–O(3)	87.1 (.3)	C(1)–C(2)–C(3)	121.0 (1.)
Co–C(13)	1.890 (.010)	N(2)–Co–O(3)	90.3 (.3)	C(2)–C(3)–C(4)	127.0 (1.)
N(1)–C(4)	1.318 (.013)	O(1)–Co–O(3)	86.6 (.3)	N(1)–C(4)–C(3)	121.5 (.9)
N(1)–C(6)	1.476 (.015)	O(2)–Co–O(3)	88.9 (.3)	N(1)–C(4)–C(5)	120.7 (1.)
N(2)–C(7)	1.466 (.013)	N(1)–Co–C(13)	93.1 (.4)	C(3)–C(4)–C(5)	117.8 (.9)
N(2)–C(9)	1.299 (.012)	N(2)–Co–C(13)	89.9 (.4)	N(1)–C(6)–C(7)	106.5 (.8)
O(1)–C(2)	1.301 (.013)	O(1)–Co–C(13)	93.2 (.4)	N(2)–C(7)–C(6)	107.4 (.8)
O(2)–C(11)	1.290 (.012)	O(2)–Co–C(13)	90.9 (.4)	N(2)–C(9)–C(8)	122.5 (.9)
C(1)–C(2)	1.518 (.017)	O(3)–Co–C(13)	179.7 (.4)	N(2)–C(9)–C(10)	122.0 (1.)
C(2)–C(3)	1.357 (.015)	Co–N(1)–C(4)	126.4 (.8)	C(8)–C(9)–C(10)	115.5 (.9)
C(3)–C(4)	1.423 (.016)	Co–N(1)–C(6)	112.3 (.6)	C(9)–C(10)–C(11)	122.5 (.9)
C(4)–C(5)	1.517 (.016)	C(4)–N(1)–C(6)	120.5 (.8)	O(2)–C(11)–C(10)	126.2 (.9)
C(6)–C(7)	1.528 (.014)	Co–N(2)–C(7)	111.0 (.6)	O(2)–C(11)–C(12)	115.2 (.9)
C(8)–C(9)	1.512 (.017)	Co–N(2)–C(8)	128.0 (.7)	C(10)–C(11)–C(12)	118.6 (.9)
C(9)–C(10)	1.458 (.015)	C(7)–N(2)–C(9)	120.9 (.9)	Co–C(13)–C(14)	127.2 (.9)
C(10)–C(11)	1.389 (.015)				
C(11)–C(12)	1.508 (.015)				
C(13)–C(14)	1.333 (.015)				

Table VI. Equations of least-squares planes and distances of atoms (in Å) from these planes

(1) Plane through Co, O(1), O(2), N(1), and N(2)

$5.206x-5.737y+7.426z=1.653$

Co	0.048 Å	O(2)	−0.019	N(2)	−0.004
O(1)	−0.005	N(1)	−0.020		

(2) Plane through O(1), N(1), C(1), C(2), C(3), C(4), C(5), and C(6)

$5.435x-5.444y+7.274z=1.699$

O(1)	−0.018 Å	C(2)	−0.010	C(5)	0.010
N(1)	−0.068	C(3)	−0.033	C(6)	0.077
C(1)	0.062	C(4)	−0.019		

(3) Plane through O(2), N(2), C(7), C(8), C(9), C(10), C(11), and C(12)

$6.044x-2.796y+7.342z=1.309$

O(2)	−0.001 Å	C(8)	−0.090	C(11)	0.030
N(2)	0.116	C(9)	0.060	C(12)	−0.142
C(7)	−0.124	C(10)	0.152		

(4) Plane through Co, O(1), O(2), N(1), N(2), C(1), C(2), C(3), C(4), C(5), C(6), C(7), C(8), C(9), C(10), C(11), C(12)

$5.306x-5.008y+7.615z=1.778$

Co	−0.032 Å	C(2)	−0.025	C(8)	0.059
O(1)	−0.062	C(3)	0.010	C(9)	0.059
O(2)	−0.201	C(4)	0.064	C(10)	0.278
N(1)	−0.001	C(5)	0.156	C(11)	0.051
N(2)	−0.111	C(6)	0.186	C(12)	0.032
C(1)	0.009	C(7)	−0.473		

double bond character. Thus it is difficult to asses the possible contribution of π-bonding to the total bond order. However, the crystallographic analyses of related complexes currently under investigation in this laboratory might offer the opportunity to elucidate the nature of the Co–C bond. The orientation of the vinyl group is such that C(14) is arranged above the acetylacetoneiminato ring Co, O(1), C(2), C(3), C(4), N(1). The dihedral angle between the planes through Co, C(13), C(14), and C(13), Co, O(1) is 36.2°.

The geometry of the equatorial tetradentate ligand was analysed by considering the equations of the best planes given in Table VI together with the distances of the individual atoms from these planes. The least-squares planes were calculated according to Shomaker *et al.*[9] with unitary weights for all the atoms. The equations are referred to the crystal axes and x, y, z are fractional coordinates. The best planes passing through the two halves of the chelate make a dihedral angle of 11.2°. The deviation from the planarity of the chelate is caused by the gauche conformation of the ethylenediamine bridge. The dihedral angle between the planes passing through N(1)–C(6)–C(7) and C(6)–C(7)–N(2) is 42.6°. Although the parent compound CoBAE has an exact tetracoordinate planar geometry, bond lengths and angles of the quadridentate ligand for the two compounds agree within twice the standard deviations.

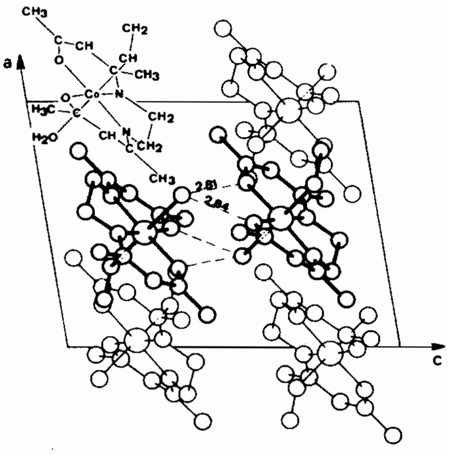

Figure 2. Projection of the structure on (010).

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(9) V. Shomaker, J. Waser, R. E. Marsh, and G. Bergman, *Acta Cryst.*, *12*, 600 (1959).

Table VII. Non-bonded distances below 4 Å

Intramolecular distances

Co—C(14)	2.897 Å	O(1)—C(14)	3.059	C(3)—C(14)	3.629
N(1)—C(14)	3.233	O(2)—C(14)	3.800	C(4)—C(14)	3.546
N(2)—C(14)	3.909	C(2)—C(14)	3.413	C(6)—C(14)	3.929

Intermolecular distances

O(1)—O(3)I	2.809 Å	C(1)—C(10)I	3.972	C(5)—C(9)III	3.807
O(2)—O(3)I	2.839	C(1)—C(11)I	3.662	C(6)—C(10)III	3.953
Co—O(3)I	3.837	C(1)—C(12)I	3.898	C(7)—C(12)III	3.848
O(1)—O(2)I	3.394	C(2)—C(11)I	3.752	C(5)—C(2)IV	3.897
O(1)—C(11)I	3.971	C(2)—C(12)I	3.722	C(9)—C(12)V	3.807
O(2)—C(11)I	3.605	C(3)—C(12)I	3.765	C(5)—O(3)VI	3.925
O(2)—C(1)I	3.831	O(2)—C(5)II	3.749	C(6)—C(13)VII	3.874
O(3)—O(3)I	3.770	C(11)—C(3)II	3.695	C(7)—C(13)VII	3.964
O(3)—C(2)I	3.688	C(12)—C(3)II	3.565	C(7)—C(14)VII	3.837
O(3)—C(1)I	3.715	C(12)—C(4)II	3.904	C(9)—C(14)VII	3.892
O(3)—C(11)I	3.795	C(12)—C(5)II	3.823	C(14)—C(9)VIII	3.941
O(3)—C(12)I	3.859	C(13)—C(3)II	3.892		

Asymmetric units

No label	x	y	z				
I	—x	—y	—z	V	—½+x	—½—y	½+z
II	—½—x	—½+y	½—z	VI	½+x	½—y	½+z
III	—½—x	½+y	½—z	VII	—x	—y	1—z
IV	—½+x	½—y	½+z	VIII	1+x	y	z

The mean Co—N bond length (1.89 Å) agrees with the value of 1.87 Å found in CoBAE, while the mean Co—O bond length (1.92 Å) is significantly greater than the value of 1.85 Å found in CoBAE. The hydrogen bonds, in which the coordinated oxygen atoms are involved, may contribute to the lengthening of the equatorial Co—O bonds. In fact pairs of molecules related by a symmetry centre make intermolecular O ..... O contacts which are of the right order for hydrogen bond formation. The oxygen atoms O(1) and O(2) are at 2.81 and 2.84 Å from the oxygen atom of the water molecule of another complex molecule, as can be seen in Figure 2 where the projection of the structure down the b-axis is shown. The arrangement of the oxygen atoms involved in the hydrogen bond formation implies that one of the lone-pairs of the water molecule is directed toward the metal atom and the other lone-pair is not specifically directed. Thus the O(1) ..... H—O'(3) and O(2) ..... H—O'(3) hydrogen bonds are bent, the angles O ..... H—O being 141.3° and 142.7° respectively. This orientation of the water molecule is consistent with the difference Fourier map which shows positive regions of the electron density in the postulated positions for the hydrogen atoms.

Non-bonded intramolecular distances and intermolecular distances below 4 Å are given in Table VII.

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