These hydrogen bonds bind the molecules into layers parallel to the (100) plane. The layers are held together by van der Waals interaction between methyl groups.

I am grateful to Professor L. Sosnowski and Professor J. Auleytner for discussion and to Dr E. Grochowski from the Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, for specimen material, discussions and cooperation.

Reference

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The crystal structure of the form of *N,N'*-ethylenebis(salicylaldehydeiminato)cobalt (II) inactive towards oxygenation.

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The structure of *N,N'*-ethylenebis(salicylaldehydeiminato)cobalt(II), $CoO_2N_2C_{16}H_{14}$, (inactive form towards oxygenation) has been refined with three-dimensional data, starting from the final coordinates obtained from the two-dimensional analysis of the isostructural analogous copper derivative. The refinement gave an R index of 0·07 for 762 independent reflexions collected on equi-inclination Weissenberg photographs taken with Mo $K\alpha$ radiation.

Introduction

One of the best known examples of synthetic molecular oxygen-carriers is *N,N'*-ethylenebis(salicylaldehydeiminato)cobalt(II) (Cosalen) which absorbs molecular oxygen reversibly in the solid state as well as in solution (Bayer & Schretzmann, 1967). Several active (oxygen-carriers) crystalline modifications and one inactive modification of this compound are known. An X-ray powder spectrum analysis was carried out by Calvin (Martell & Calvin, 1959). However, the mode of attachment of oxygen and the absorption mechanism in the solid phase are still subjects of discussion. As part of a general investigation of these two aspects, we present here the three-dimensional analysis of the inactive form.

This work was carried out in order to obtain more accurate values of bond lengths and angles for subsequent comparison with the analogous compound $(Cosalen)_2 . (dimethylformamide)_2 . O_2$, under investigation in this laboratory. The crystal structure of this compound will be described in a forthcoming paper. Dr S. Holt and his co-workers (private communication) have independently refined the structure of inactive Cosalen and their results agree with ours.

Experimental

The crystals, prepared according to Bailes & Calvin (1947), are monoclinic with $a = 26{\cdot}52 \pm 0{\cdot}03$, $b = 7{\cdot}05 \pm 0{\cdot}01$, $c = 14{\cdot}36 \pm 0{\cdot}02$ Å, $\beta = 98{\cdot}4 \pm 0{\cdot}3°$, $Z = 8$, $D_c = 1{\cdot}63$ g.cm^{-3},

Table 1. *Atomic fractional coordinates* ($\times 10^4$) *and isotropic thermal parameters with e.s.d.'s given in parentheses*

The fractional coordinates ($\times 10^3$) of the hydrogen atoms are listed near their bonded carbon atoms.

	x	y	z	B		x	y	z
Co	2340 (1)	2034 (3)	977 (1)	1·68 (3)				
O(1)	1869 (4)	4043 (14)	901 (6)	2·32 (20)				
O(2)	2833 (3)	3773 (13)	554 (6)	1·65 (18)				
N(1)	1910 (4)	407 (17)	1532 (7)	1·83 (25)				
N(2)	2830 (5)	107 (19)	1259 (8)	2·20 (27)				
C(1)	1376 (5)	3995 (23)	1044 (9)	2·34 (33)				
C(2)	1076 (6)	5617 (24)	795 (10)	2·95 (36)	H(1)	124	686	49
C(3)	573 (6)	5629 (24)	940 (11)	3·25 (37)	H(2)	34	691	78
C(4)	350 (6)	4028 (27)	1277 (11)	3·73 (40)	H(3)	−6	46	134
C(5)	632 (6)	2423 (24)	1519 (11)	3·54 (39)	H(4)	45	120	180
C(6)	1163 (5)	2335 (21)	1397 (9)	2·33 (33)				
C(7)	1436 (6)	680 (24)	1655 (10)	2·86 (35)	H(5)	124	−46	198
C(8)	2172 (5)	−1294 (21)	1937 (9)	2·27 (31)	H(6)	231	−107	267
					H(7)	190	−248	188
C(9)	2610 (5)	−1733 (22)	1391 (10)	2·50 (32)	H(8)	248	−240	72
					H(9)	289	−267	178
C(10)	3336 (5)	335 (22)	1414 (10)	2·32 (33)	H(10)	357	−87	166
C(11)	3573 (5)	2099 (23)	1267 (9)	2·17 (28)				
C(12)	4128 (6)	2131 (28)	1557 (11)	3·64 (37)	H(11)	431	89	188
C(13)	4375 (6)	3790 (27)	1397 (11)	3·81 (41)	H(12)	479	384	161
C(14)	4148 (6)	5370 (23)	995 (11)	2·99 (37)	H(13)	437	660	87
C(15)	3607 (6)	5361 (24)	723 (10)	2·90 (35)	H(14)	340	664	44
C(16)	3335 (5)	3664 (20)	844 (9)	1·71 (28)				

Table 2. *Observed and calculated structure factors*

H	K	|FO|	|FC|
••••••L=		0•••••	
2	0	383	363
2	2	75	87
2	6	42	43
3	1	70	64
3	3	39	41
4	0	47	49
4	2	150	148
4	6	48	46
5	3	118	118
6	0	183	178
6	2	190	192
6	4	65	63
7	1	58	52
7	3	143	137
8	2	134	143
8	4	47	49
9	1	48	48
9	3	90	91
9	5	46	46
10	0	148	129
10	2	91	89
11	1	52	43
11	3	98	110
11	5	44	43
12	2	60	61
13	1	91	86
13	3	88	98
14	0	62	55
15	3	103	108
15	5	62	55
17	3	101	104
17	5	82	80
19	5	85	87
20	0	70	53
21	5	62	74
22	0	82	75
24	0	83	79
••••••L=		1•••••	
0	6	128	142
1	1	285	290
-1	-1	255	253
-2	-4	54	58
2	6	67	67
-2	-6	70	60
3	1	97	99
-3	-1	65	64
3	3	57	43
3	5	57	54
4	2	77	65
-4	-2	47	31
-4	-4	103	115
-4	-6	40	33
5	1	128	117
-5	-1	35	33
5	3	92	96
-5	-3	78	73
6	2	40	39
-6	-2	135	125
-6	-4	101	108
-6	-6	61	63
7	1	72	70
7	3	229	239
-7	-3	51	46
8	2	58	56
-8	-2	138	137
-8	-4	95	101
-8	-6	54	52
9	1	130	122
9	3	105	102
10	2	60	51
-10	-2	84	91
10	4	52	48
-10	-4	92	95
-10	-6	67	73
11	1	133	129
-11	-1	35	37
11	3	101	101

H	K	|FC|	|FO|
12	2	64	54
-12	-2	115	125
12	4	57	61
-12	-4	71	75
-13	-1	36	32
13	3	69	64
-13	-3	42	41
14	2	62	57
-14	-2	66	70
14	4	72	75
-14	-4	82	91
15	1	50	44
-15	-1	64	66
15	3	59	59
-15	-3	48	51
16	2	88	81
-16	-2	87	94
16	4	69	70
-16	-4	58	64
16	6	67	66
-16	-6	51	48
17	1	81	76
-17	-1	93	101
17	3	86	80
-17	-3	98	104
18	2	42	30
-18	-2	50	49
18	4	66	70
-18	-4	66	71
18	6	64	63
-18	-6	54	47
19	1	42	44
-19	-1	106	117
19	3	54	43
20	2	45	34
20	4	88	85
20	6	65	61
-21	-1	99	109
-21	-3	48	39
22	2	47	42
22	4	56	42
22	6	67	73
-23	-1	96	103
-23	-3	50	46
24	2	59	47
24	4	54	47
24	6	58	56
-25	-1	75	83
-27	-3	64	51
••••••L=		2•••••	
0	0	95	99
1	1	74	75
-1	-1	30	30
1	3	63	65
-1	-3	68	74
1	5	149	166
-1	-5	173	199
1	7	65	66
-1	-7	43	51
2	0	147	135
-2	-0	28	25
2	2	82	85
-2	-2	55	33
2	6	55	55
-2	-6	45	51
3	1	236	225
-3	-1	225	231
3	3	28	25
-3	-3	60	67
3	5	72	66
-3	-5	106	104
3	7	37	40
-3	-7	33	28
4	0	54	47
4	2	97	98
-4	-2	34	35
-4	-4	36	32
5	3	86	84

H	K	|FO|	|FC|
-5	-3	134	146
5	5	70	77
-5	-5	83	93
-5	-7	33	29
6	0	127	126
-6	-0	78	73
6	2	66	71
-6	-2	76	77
6	4	65	59
7	1	54	49
-7	-1	59	53
7	3	133	132
-7	-3	197	210
7	5	31	31
-7	-5	59	62
-7	-7	44	53
8	0	94	96
8	2	147	144
-8	-2	89	89
8	4	59	69
-9	-1	38	39
9	3	59	59
-9	-3	107	119
9	5	28	31
-9	-5	61	66
-9	-7	58	54
10	0	176	167
-10	-0	134	135
10	2	129	130
-10	-2	69	74
10	4	32	32
-11	-1	32	32
11	3	39	35
-11	-3	73	78
-11	-5	47	52
-11	-7	42	49
12	2	127	132
-12	-2	102	108
12	4	36	38
13	1	46	40
-13	-1	73	69
-13	-3	59	62
-13	-5	39	35
-14	-0	54	54
14	2	117	118
-14	-2	87	100
15	1	54	51
15	3	27	31
-15	-3	44	40
16	0	122	116
-16	-0	137	145
16	2	86	89
-16	-2	87	103
16	4	65	60
-16	-4	67	65
-17	-3	37	44
18	0	95	103
-18	-0	132	149
18	2	74	67
-18	-2	78	84
18	4	46	57
-18	-4	41	46
19	5	44	51
20	0	80	84
-20	-0	115	125
21	3	40	39
21	5	46	61
22	0	89	87
-22	-0	127	142
23	3	44	56
23	5	54	52
24	0	61	54
-24	-0	86	92
-24	-2	44	41
25	3	46	48
25	5	45	41
-26	-2	44	52
27	3	44	45

H	K	|FO|	|FC|
••••••L=		3•••••	
0	2	24	27
0	4	75	83
0	6	135	161
1	1	82	80
-1	-1	115	115
1	5	63	56
-1	-5	83	82
2	4	81	95
-2	-4	103	124
2	6	91	90
-2	-6	82	78
3	1	201	191
-3	-1	119	106
-3	-5	45	39
-4	-2	47	49
4	4	52	102
-4	-4	89	104
4	6	72	68
5	1	83	77
-5	-1	86	86
5	3	40	30
-5	-3	65	70
6	2	112	115
-6	-2	138	142
6	4	75	75
6	6	79	77
7	1	91	83
-7	-1	101	104
-7	-3	160	182
8	2	70	70
-8	-2	114	110
8	4	85	88
8	6	64	62
9	1	99	91
-9	-1	165	156
9	3	83	79
-9	-3	70	65
-10	-2	58	53
10	4	85	77
10	6	78	78
11	1	61	62
-11	-1	160	154
11	3	81	72
-11	-3	81	77
12	2	60	48
13	1	88	85
-13	-1	78	81
13	3	77	80
-13	-3	67	67
14	4	39	46
15	1	75	75
-15	-1	114	114
15	3	94	98
-15	-3	75	75
16	4	65	57
-16	-4	48	55
17	1	84	78
-17	-1	125	135
17	3	106	109
-17	-3	82	81
-18	-2	63	66
19	1	111	115
-19	-1	119	130
-19	-3	53	48
21	1	83	90
-21	-1	80	89
-22	-2	65	72
23	1	66	76
-24	-2	52	63
25	1	60	67
••••••L=		4•••••	
0	0	571	627
0	2	41	43
0	4	64	64
1	1	229	238
-1	-1	172	168
1	3	43	39

H	K	|FO|	|FC|
-1	-3	38	35
1	5	95	107
-1	-5	83	77
2	0	180	172
-2	-0	117	122
-2	-2	73	83
2	4	66	61
-2	-4	59	55
3	1	32	33
-3	-1	87	87
3	5	91	94
-3	-5	68	69
4	0	90	89
-4	-0	44	28
-4	-2	109	124
-4	-4	62	64
5	1	39	34
-5	-1	153	138
5	3	83	76
5	5	70	75
6	0	78	75
-6	-0	135	138
6	2	114	97
-6	-2	137	153
-6	-4	97	99
7	1	63	57
-7	-1	34	32
7	3	109	101
7	5	65	65
-8	-0	82	88
8	2	75	57
-8	-2	162	183
-8	-4	72	74
9	1	39	32
-9	-1	47	41
9	3	85	81
9	5	69	75
10	0	78	76
-10	-0	140	141
-10	-2	140	149
10	4	67	55
-11	-1	59	53
11	3	93	92
-11	-5	52	37
-12	-0	49	50
-12	-2	106	110
13	1	73	61
13	3	73	72
-13	-3	39	40
14	0	56	55
-14	-0	69	69
14	2	61	57
-14	-2	86	96
14	4	80	74
15	3	91	84
-15	-3	48	45
-15	-5	57	49
16	0	88	82
-16	-0	144	136
16	4	51	47
17	3	96	94
-17	-3	62	58
-17	-5	74	72
18	0	84	85
-18	-0	88	95
-19	-5	84	79
20	0	84	93
-20	-0	48	48
20	2	85	94
-20	-2	67	68
-21	-5	66	64
22	0	110	115
-23	-3	59	54
-23	-5	69	60
24	0	88	97
••••••L=		5•••••	
0	2	32	30
1	1	239	251

H	K	|FO|	|FC|
-1	-1	206	199
1	3	38	42
-1	-3	60	63
2	2	79	80
-2	-2	69	67
2	4	95	105
3	1	174	179
-3	-1	161	160
-3	-3	50	49
4	2	31	34
4	4	110	107
-4	-4	31	36
5	1	97	94
-5	-1	45	45
5	3	50	47
-5	-3	100	108
6	2	113	114
6	4	42	43
-6	-4	72	80
6	6	50	46
7	1	84	80
-7	-1	42	46
7	3	109	100
-7	-3	97	107
8	2	120	123
-8	-2	68	69
8	4	50	46
-8	-4	75	78
8	6	67	60
9	1	122	113
-9	-1	54	51
10	2	96	95
10	4	80	71
-10	-4	70	69
10	6	54	51
11	1	76	67
-11	-3	54	55
12	2	74	78
-12	-2	79	78
12	4	84	81
-12	-4	58	58
14	2	96	97
-14	-2	49	55
14	4	93	90
-14	-4	87	81
16	2	107	109
-16	-2	70	74
16	4	75	60
-16	-4	50	45
-17	-3	57	55
18	4	55	63
-18	-4	74	68
19	1	44	47
20	4	75	72
-20	-4	95	87
21	1	73	70
-23	-3	66	44
••••••L=		6•••••	
0	0	150	151
1	1	118	112
-1	-1	70	50
1	3	35	31
-1	-3	50	48
1	5	56	53
-1	-5	124	122
2	0	143	153
-2	-0	130	130
2	2	129	150
-2	-2	111	121
3	1	116	112
-3	-1	87	96
-3	-3	67	71
-3	-5	86	70
4	0	97	102
-4	-0	73	70
4	2	119	136
-4	-2	107	109
-4	-4	67	73

H	K	|FO|	|FC|
-5	-3	98	103
-5	-5	75	61
6	0	118	118
-6	-0	35	33
6	2	45	46
-6	-2	51	37
6	4	51	48
-6	-4	64	61
-7	-1	31	36
-7	-3	126	140
-7	-5	63	70
8	0	107	95
-8	-0	80	70
8	2	128	124
8	4	59	61
-8	-4	47	41
-9	-1	40	38
-9	-3	99	104
-9	-5	84	92
10	0	128	117
-10	-0	39	29
10	2	83	86
-11	-3	83	63
-11	-5	73	76
12	0	44	47
12	2	66	60
13	1	82	81
-13	-1	98	100
-13	-3	79	83
-13	-5	70	58
-14	-0	43	38
14	2	68	67
15	1	77	79
-15	-1	46	50
15	3	66	62
-15	-3	93	60
-16	-0	64	62
16	2	44	45
-16	-2	74	78
17	3	56	48
-17	-3	64	72
-18	-0	78	83
-18	-2	46	46
-20	-0	87	65
-22	-0	91	93
-24	-0	78	75
••••••L=		7•••••	
0	2	40	44
0	4	88	91
1	1	46	47
1	5	70	67
-1	-5	64	53
2	2	53	60
-2	-2	62	72
2	4	77	74
-2	-4	118	124
3	1	198	199
-3	-1	117	119
4	2	81	87
-4	-2	94	97
-4	-4	100	105
5	1	109	111
5	3	46	38
6	2	85	88
-6	-2	110	118
7	1	119	125
-7	-1	86	84
-8	-2	56	59
-8	-4	74	72
9	1	134	139
-9	-1	107	103
9	3	43	58
-10	-2	37	42
-10	-4	66	59
11	1	95	98
-11	-1	51	64
11	3	63	48
13	1	108	109

H	K	|FO|	|FC|
-13	-1	37	40
13	3	54	50
-13	-3	61	48
14	2	67	65
15	1	74	81
-15	-1	98	94
15	3	56	53
-15	-3	58	58
16	2	59	59
-17	-1	92	85
17	3	58	46
-17	-3	76	72
-18	-2	67	69
-19	-1	91	97
-21	-1	78	79
-23	-3	53	58
••••••L=		8•••••	
0	4	65	53
1	1	111	98
-1	-1	46	38
1	3	93	89
-1	-3	96	92
1	5	79	77
-1	-5	84	71
2	0	41	46
2	4	77	76
-3	-1	129	128
3	3	67	63
-3	-3	70	69
-3	-5	74	77
-4	-0	74	76
4	2	77	75
-5	-1	148	147
5	3	60	61
-5	-3	79	75
6	0	66	67
-6	-0	115	133
-6	-2	67	69
7	1	54	56
-7	-1	56	53
-7	-3	58	47
8	0	77	79
-8	-0	123	131
-8	-2	133	141
-9	-1	63	62
10	0	46	50
-10	-0	164	158
-10	-2	97	102
11	1	58	56
-11	-1	65	62
12	0	79	72
-12	-0	121	128
12	2	69	61
-12	-2	72	70
14	0	72	67
-14	-0	114	124
14	2	81	81
-14	-2	95	103
14	4	65	72
16	0	75	73
-16	-0	128	132
-16	-2	56	56
16	4	58	62
-17	-1	67	66
18	0	55	58
-18	-0	86	99
-18	-2	58	64
20	0	57	58
-20	-0	60	61
20	2	66	73
-20	-2	106	114
-22	-0	63	58
••••••L=		9•••••	
0	4	40	41
1	1	70	72
-1	-1	69	64
1	3	55	54
-1	-3	60	58

H	K	|FO|	|FC|
2	2	56	52
2	4	121	120
-2	-4	63	57
3	1	46	51
-3	-1	110	104
-3	-3	69	60
4	2	33	36
-4	-2	73	77
4	4	107	103
-4	-4	40	46
-5	-1	59	61
-5	-3	55	64
6	2	93	91
-6	-2	74	85
6	4	51	52
6	6	65	61
-7	-1	84	85
-7	-3	61	57
8	2	60	64
8	4	68	61
8	6	66	58
9	1	50	40
-9	-1	114	114
-9	-3	57	60
-10	-2	47	46
10	4	63	52
10	6	63	55
-11	-1	74	72
-11	-3	52	58
12	4	46	52
12	6	65	50
-13	-1	91	94
14	4	58	59
16	2	49	50
-19	-1	55	61
••••••L=		10••••••	
0	0	70	64
0	2	51	49
1	1	56	57
2	0	60	57
-2	-0	110	115
2	2	109	118
-2	-2	90	93
-2	-4	42	27
4	0	47	48
-4	-0	113	115
4	2	79	87
-4	-2	83	82
-4	-4	78	70
5	3	60	56
-6	-0	107	99
-6	-4	67	63
7	3	55	47
-8	-0	89	98
8	2	52	60
-9	-3	53	53
-10	-0	67	57
-10	-2	55	53
-11	-3	72	61
-12	-0	69	64
-12	-2	47	50
-13	-1	52	60
-13	-3	62	63
15	1	58	57
-15	-1	62	69
-15	-3	76	67
-17	-3	66	65
-19	-3	68	61
-21	-3	70	60
22	0	64	69
-23	-3	56	44
••••••L=		11••••••	
0	4	54	53
1	1	66	67
-1	-1	66	57
-1	-3	54	53
-2	-4	54	53
3	1	96	106

H	K	|FO|	|FC|
-3	-1	88	99
3	3	62	55
-3	-3	47	34
4	2	41	43
5	1	53	60
5	3	90	94
-5	-3	61	62
7	1	62	69
7	3	50	45
-8	-4	70	70
9	1	55	75
-10	-4	64	58
11	1	57	58
-12	-2	46	47
13	1	59	70
-14	-2	54	51
-16	-2	48	44
••••••L=		12••••••	
0	0	66	54
1	3	64	60
-1	-3	64	59
2	0	67	62
-3	-1	62	51
3	3	50	54
-3	-3	57	49
4	0	52	53
-4	-0	72	67
4	2	67	74
5	3	51	48
-5	-3	49	49
6	0	69	69
-6	-0	51	51
6	2	62	71
-8	-0	51	54
8	2	57	59
-8	-2	57	57
10	0	79	78
-10	-0	67	67
12	0	117	125
-12	-0	69	64
14	0	84	86
-14	-2	56	63
16	0	61	64
-16	-2	50	57
-18	-2	51	60
-20	-2	83	87
••••••L=		13••••••	
0	4	48	46
-2	-2	48	52
2	4	85	76
-2	-4	68	62
-3	-1	65	53
-4	-2	78	68
4	4	49	50
-4	-4	68	64
-5	-1	56	49
6	2	54	61
-6	-2	76	69
-7	-1	65	65
-9	-1	105	83
-11	-1	58	63
-13	-1	76	67
••••••L=		14••••••	
-2	-0	65	70
-4	-0	92	96
5	3	65	65
-6	-0	80	83
-8	-0	80	75
-10	-0	57	70
-12	-0	58	68
••••••L=		15••••••	
-1	-1	62	61
-3	-1	79	78
-5	-1	71	65
5	3	58	71
-7	-1	62	63

Table 3. *Bond lengths and angles*

Standard deviations are given in parentheses and refer to the last significant figures.

Co—O(1)	1·88 (1) Å	Co—N(1)—C(7)	128·5 (11)°
Co—O(2)	1·95 (1)	Co—N(1)—C(8)	112·8 (8)
Co—N(1)	1·88 (1)	C(7)—N(1)—C(8)	118·5 (12)
Co—N(2)	1·88 (1)	Co—N(2)—C(9)	113·4 (9)
O(1)—C(1)	1·35 (2)	Co—N(2)—C(10)	126·4 (11)
O(2)—C(16)	1·34 (2)	C(9)—N(2)—C(10)	120·0 (13)
N(1)—C(7)	1·31 (2)	O(1)—C(1)—C(2)	117·6 (14)
N(1)—C(8)	1·46 (2)	O(1)—C(1)—C(6)	121·1 (13)
N(2)—C(9)	1·45 (2)	C(2)—C(1)—C(6)	121·2 (13)
N(2)—C(10)	1·34 (2)	C(1)—C(2)—C(3)	119·3 (15)
C(1)—C(2)	1·41 (2)	C(2)—C(3)—C(4)	121·1 (15)
C(2)—C(3)	1·38 (2)	C(3)—C(4)—C(5)	120·8 (15)
C(3)—C(4)	1·39 (3)	C(4)—C(5)—C(6)	120·6 (15)
C(4)—C(5)	1·37 (2)	C(1)—C(6)—C(5)	116·9 (13)
C(5)—C(6)	1·45 (2)	C(5)—C(6)—C(7)	118·7 (14)
C(6)—C(7)	1·39 (2)	C(1)—C(6)—C(7)	124·4 (13)
C(8)—C(9)	1·53 (2)	N(1)—C(7)—C(6)	124·0 (15)
C(10)-C(11)	1·43 (2)	N(1)—C(8)—C(9)	108·4 (11)
C(11)-C(12)	1·47 (2)	N(2)—C(9)—C(8)	103·7 (12)
C(12)-C(13)	1·38 (3)	N(2)—C(10)-C(11)	122·5 (13)
C(13)-C(14)	1·36 (2)	C(10)-C(11)-C(12)	114·8 (14)
C(14)-C(15)	1·43 (2)	C(10)-C(11)-C(16)	125·5 (12)
C(15)-C(16)	1·42 (2)	C(12)-C(11)-C(16)	119·6 (14)
		C(11)-C(12)-C(13)	116·5 (15)
O(1)-Co—O(2)	88·8 (4)°	C(12)-C(13)-C(14)	125·3 (15)
O(1)-Co—N(1)	92·6 (5)	C(13)-C(14)-C(15)	118·6 (15)
O(2)-Co—N(2)	92·7 (5)	C(14)-C(15)-C(16)	118·5 (14)
N(1)-Co—N(2)	84·9 (5)	C(11)-C(16)-C(15)	121·4 (13)
Co —O(1)-C(1)	128·4 (10)	O(2)—C(16)-C(11)	124·1 (13)
Co —O(2)-C(16)	123·2 (8)	O(2)—C(16)-C(15)	141·4 (12)

$D_m = 1\cdot60$ g.cm^{-3} (values previously reported by Martell & Calvin (1959): $a = 14\cdot07$, $b = 7\cdot06$, $c = 26\cdot25$, $\beta = 97\cdot75°$). With our choice of axes the possible space groups are *Cc* or *C*2/*c*. The latter has been chosen, because this compound was found to be isostructural with the analogous copper derivative (Hall & Waters, 1960). This choice was later verified by the successful refinement of the structure.

Intensity data were collected by the equi-inclination Weissenberg method with Mo *Kα* radiation. Levels *h*0*l* through *h*6*l* and *hk*0 through *hk*2 were recorded by the multiple film technique. The intensities were measured visually by comparison with a series of calibrated spots. Lorentz and polarization factors and the spot-shape correction (Phillips, 1954) for non-zero levels were applied. No correction for absorption was made ($\mu = 13\cdot4$ cm^{-1} for Mo *Kα* and $\mu R \sim 0\cdot2$). The data were scaled by the method of Hamilton, Rollett & Sparks (1965). The number of independent reflexions was 762.

Initial fractional coordinates were taken from the two-dimensional analysis of the isostructural copper compound and were refined by isotropic block-diagonal least-squares method to an *R* value of 0·067. The contribution of hydrogen atoms was included, but the positions of these atoms were not refined. Their thermal motion was assumed isotropic with the same *B* values as those of the carbon atoms to which they are bonded.

No region of electron density exceeded ± 0·3 e.Å^{-3} on the final $|F_o - F_c|$ synthesis. The least-squares program was that of Albano, Domenicano & Vaciago (1966) which minimizes the function $\Sigma w(|F_o| - |F_c|)^2/\Sigma w|F_o|^2$, where F_o and F_c are the observed and calculated structure factors, respectively, and *w* is the weighting factor. The weighting scheme $w = (a + b|F_o| + c|F_o|^2)^{-1}$, with $a = 25\cdot0$, $b = 1\cdot0$, $c = 0\cdot004$, was used.

The atomic scattering factors used were those of Hanson, Herman, Lea & Skillman (1964) for oxygen, carbon and hydrogen, that of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for nitrogen and that listed in *International Tables of X-Ray Crystallography* (1962) for cobalt.

Atomic parameters and their standard deviations are given in Table 1. The final observed and calculated structure factors are listed in Table 2. A sketch of the dimer is shown in Fig. 1 with the numbering scheme for the atoms of the crystallographically independent unit. The bond lengths and angles are given in Table 3. In Table 4 are listed the distances below 4 Å within the dimer.

Table 4. *Distances below* 4 Å *within the dimer*

The primed atoms refer to the molecule at $\frac{1}{2}-x$, $\frac{1}{2}-y$, $\bar{z}$. Standard deviations are given in parentheses and refer to the last significant figure.

Co—Co′	3·118 (3) Å
Co—O(1′)	3·73 (1)
Co—O(2′)	2·25 (1)
Co—N(2′)	3·76 (1)
Co—C(11′)	3·80 (1)
Co—C(15′)	3·65 (2)
Co—C(16′)	2·99 (1)
O(1)-O(2′)	3·07 (1)
O(1)-N(2′)	3·37 (2)
O(1)-C(10′)	3·32 (2)
O(1)-C(11′)	3·26 (2)
O(1)-C(15′)	3·98 (2)
O(1)-C(16′)	3·13 (2)
O(2)-O(2′)	2·84 (1)
O(2)-N(1′)	3·22 (1)
O(2)-N(2′)	3·03 (1)
O(2)-C(1′)	3·86 (2)
O(2)-C(7′)	3·97 (2)
O(2)-C(8′)	3·99 (2)
O(2)-C(9′)	3·55 (2)
O(2)-C(10′)	3·93 (2)
O(2)-C(16′)	3·84 (2)
N(1)-C(16′)	3·44 (2)
C(1)-C(10′)	3·75 (2)
C(1)-C(11′)	3·53 (2)
C(1)-C(12′)	3·86 (2)
C(1)-C(15′)	3·99 (2)
C(1)-C(16′)	3·47 (2)
C(2)-C(10′)	3·79 (2)
C(2)-C(11′)	3·75 (2)
C(2)-C(12′)	3·86 (2)
C(6)-C(14′)	3·91 (2)
C(6)-C(15′)	3·71 (2)
C(6)-C(16′)	3·73 (2)
C(7)-C(14′)	3·96 (2)
C(7)-C(15′)	3·48 (2)
C(7)-C(16′)	3·76 (2)

Discussion

The present analysis has shown that the crystal consists of centrosymmetric dimeric units, (Cosalen)$_2$, rather than

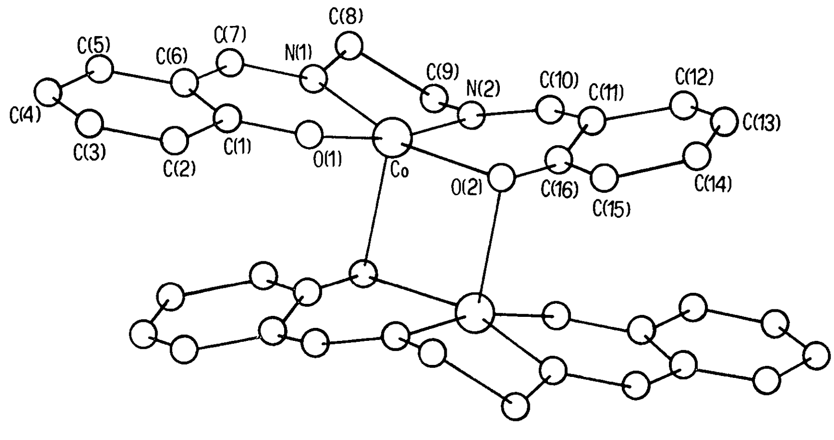

Fig. 1. The sketch of the dimer with the numbering scheme for the atoms.

of monomeric units arranged in layers, as previously proposed (Martell & Calvin, 1959). Dimerization is achieved by the sharing of one oxygen atom from each 'salen' ligand by two cobalt atoms. Thus the cobalt atom is five coordinated in a distorted rectangular based pyramid with an axial bond Co–O of 2·25 Å. The close approach of the two halves of the dimer requires the two planes of the 'salen' ligand to bend away from each other. The Co–N (mean value 1·88 Å) and Co–O (1·88 Å) bond lengths agree with the mean values of 1·88 and 1·86 Å respectively, found in some organo-cobalt derivatives of bis(acetylacetone)-ethylendiimine (BAEH$_2$), (Brückner, Calligaris, Nardin & Randaccio, 1968*a*). On the other hand, the Co–O value of 1·95 Å agrees with the mean value of 1·92 Å found in vinyl-aquo(BAE)Co (Brückner, Calligaris, Nardin & Randaccio, 1968*b*). In the last compound the lengthening of Co–O bonds has been ascribed to the intermolecular hydrogen bonds in which these oxygen atoms are involved. Analogously the lengthening found here can be ascribed to the additional coordination bond of 2·25 Å in which the oxygen atom is involved.

The torsional angle around the CH$_2$–CH$_2$ bond is 42·0° and the angle between the planes passing through the two halves of the 'salen' ligand is 22·2°. The close stacking of the dimeric units does not introduce voids in the structure. Thus the crystal packing of the inactive form is such that it may be regarded as 'self-protecting' towards oxygen absorption.

The dimeric nature of this compound suggests a possible explanation of the two-to-one stoichiometry of the oxygenated adduct. If one assumes that the crystals of the active form consist of dimers packed in an open way, the formation of an adduct [(cosalen)$_2$O$_2$]$_n$ seems likely when the oxygen molecules penetrate into the voids of the structure. On the contrary, in the model of equally displaced monomeric units, proposed by Calvin, the 2:1 and 1:1 ratios would both be possible.

However this conjecture requires further experimental information to support it.

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